



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:42 PM UTC

PDB ID : 8U29 / pdb_00008u29
EMDB ID : EMD-41842
Title : Prefusion structure of the PRD-0038 spike glycoprotein ectodomain trimer
Authors : Lee, J.; Park, Y.J.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2023-09-05
Resolution : 2.80 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

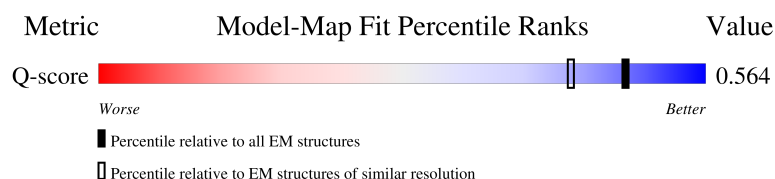
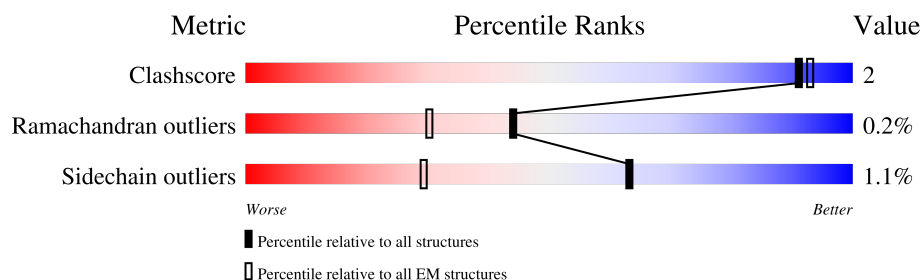
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1280	 5% 77% 7% 15%
1	B	1280	 5% 77% 7% 15%
1	C	1280	 5% 77% 7% 15%
2	D	2	 100% 100%

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Mol	Chain	Length	Quality of chain	
2	E	2	50%	100%
2	F	2	100%	100%
2	I	2	50%	100%
2	J	2	50%	100%
2	K	2	50%	100%
2	L	2	50%	100%
2	M	2	50%	100%
2	N	2	100%	100%
2	O	2	50%	100%
2	P	2	100%	100%
2	S	2	50%	100%
2	T	2	50%	100%
2	U	2	50%	100%
2	V	2	50%	100%
2	W	2	50%	100%
2	X	2	100%	100%
2	Y	2	50%	100%
2	Z	2	100%	100%
2	c	2	50%	100%
2	d	2	50%	100%
2	e	2	50%	100%
2	f	2	50%	100%
2	g	2	50%	100%
3	G	4	50%	50%
3	Q	4	100%	50%

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Mol	Chain	Length	Quality of chain
3	a	4	100% 50% 50%
4	H	6	33% 17% 83%
4	R	6	33% 17% 83%
4	b	6	33% 17% 83%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25726 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 PRD-0038 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1082	Total	C	N	O	S	0	0
			8073	5193	1371	1468	41		
1	B	1082	Total	C	N	O	S	0	0
			8075	5194	1371	1469	41		
1	C	1082	Total	C	N	O	S	0	0
			8078	5195	1371	1471	41		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		
2	f	2	Total	C	N	O	0	0
			28	16	2	10		
2	g	2	Total	C	N	O	0	0
			28	16	2	10		

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



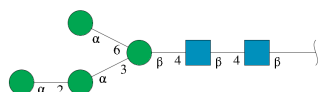
Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	4	Total	C	N	O	0	0
			50	28	2	20		

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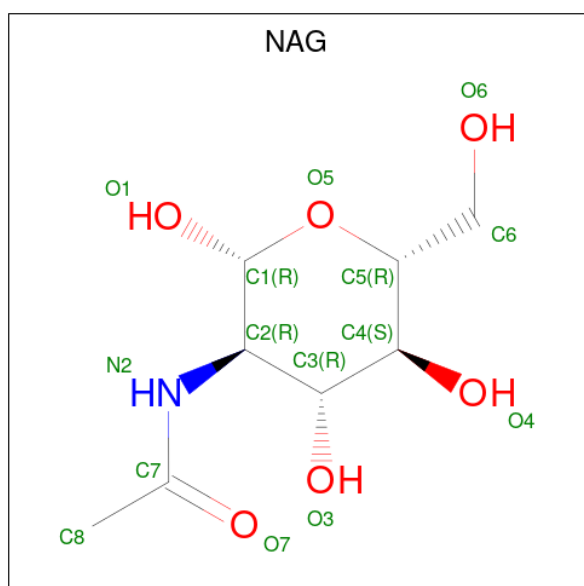
Mol	Chain	Residues	Atoms				AltConf	Trace
3	Q	4	Total	C	N	O	0	0
			50	28	2	20		
3	a	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	6	Total	C	N	O	0	0
			72	40	2	30		
4	R	6	Total	C	N	O	0	0
			72	40	2	30		
4	b	6	Total	C	N	O	0	0
			72	40	2	30		

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



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

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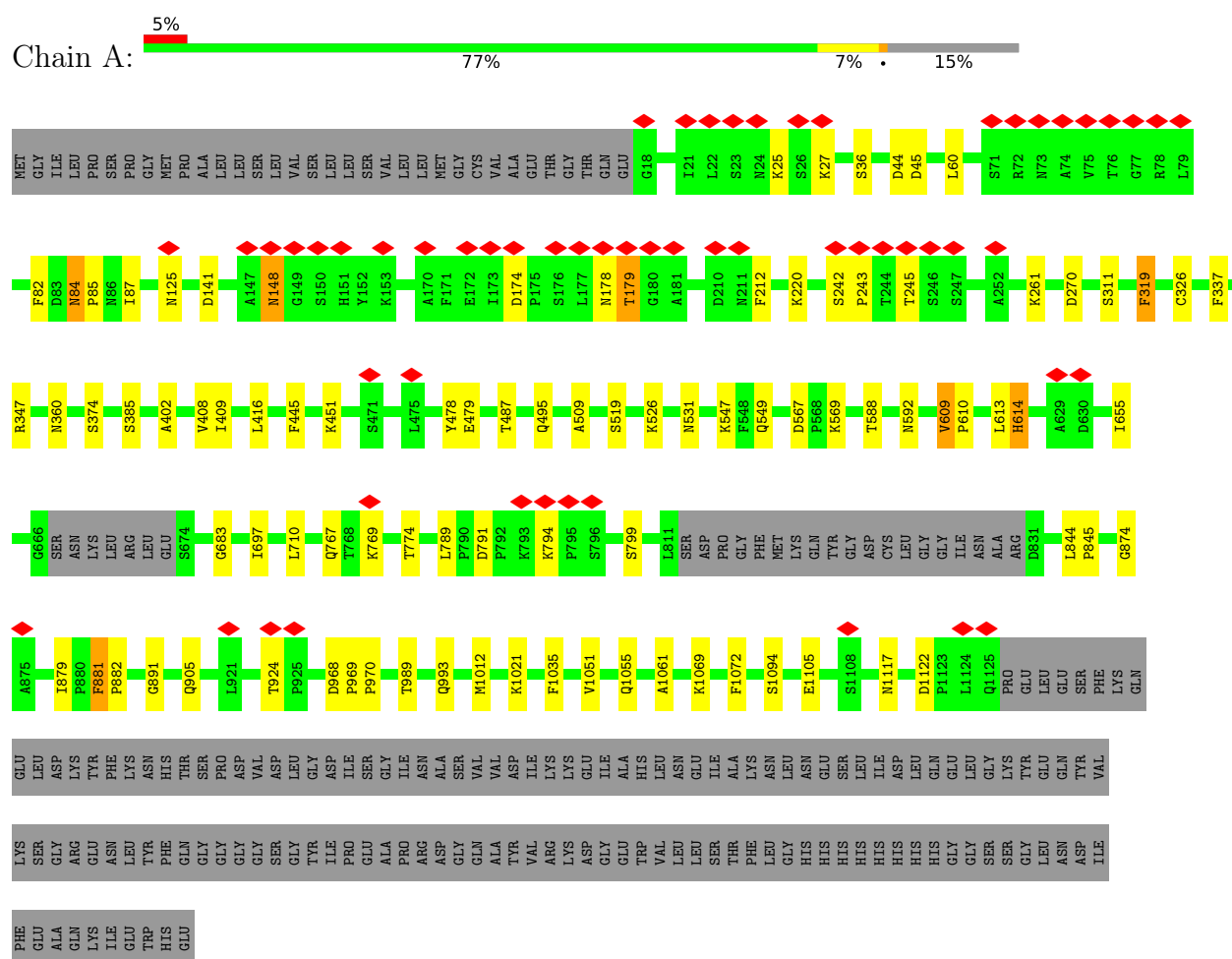
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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C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

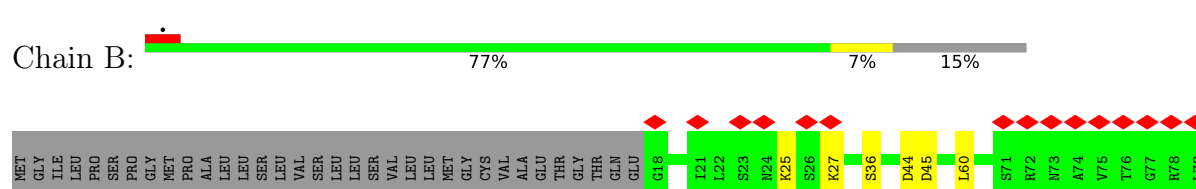
3 Residue-property plots [i](#)

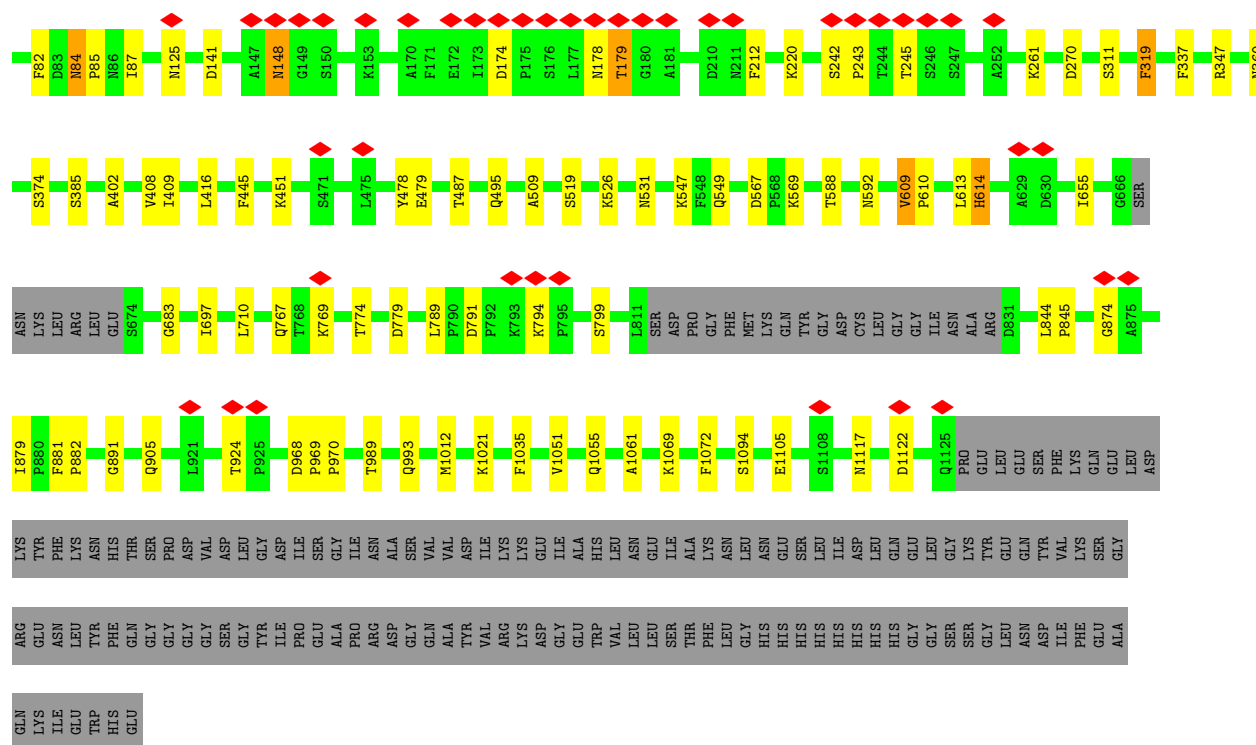
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: PRD-0038 Spike glycoprotein

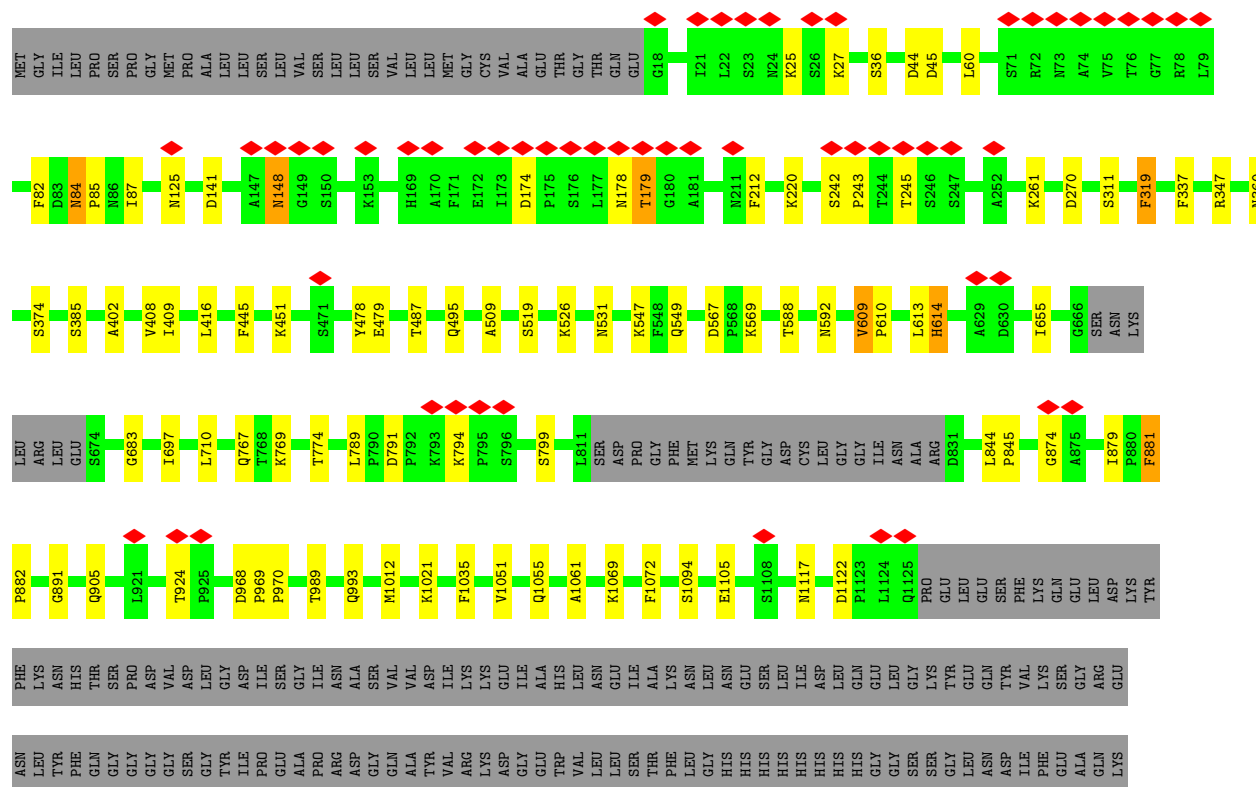
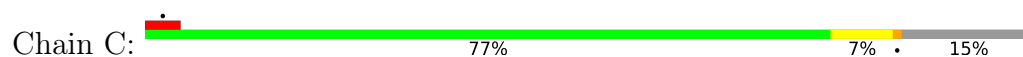


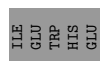
• Molecule 1: PRD-0038 Spike glycoprotein





• Molecule 1: PRD-0038 Spike glycoprotein





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



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



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



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



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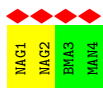




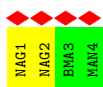
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



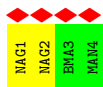
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



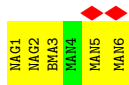
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

ido-2-deoxy-beta-D-glucopyranose



● Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	103347	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	0	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.558	Depositor
Minimum map value	-4.098	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	512.0, 512.0, 512.0	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.60	1/8267 (0.0%)	1.00	96/11288 (0.9%)
1	B	0.60	1/8269 (0.0%)	1.00	92/11291 (0.8%)
1	C	0.60	1/8272 (0.0%)	1.00	94/11295 (0.8%)
All	All	0.60	3/24808 (0.0%)	1.00	282/33874 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	ASN	C-O	-5.73	1.16	1.23
1	C	148	ASN	C-O	-5.72	1.16	1.23
1	B	148	ASN	C-O	-5.71	1.16	1.23

All (282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	614	HIS	N-CA-CB	14.79	135.49	110.49
1	B	614	HIS	N-CA-CB	14.79	135.49	110.49
1	A	614	HIS	N-CA-CB	14.79	135.48	110.49
1	C	844	LEU	CA-C-N	9.60	126.57	119.66
1	C	844	LEU	C-N-CA	9.60	126.57	119.66
1	B	844	LEU	CA-C-N	9.60	126.57	119.66
1	B	844	LEU	C-N-CA	9.60	126.57	119.66
1	A	844	LEU	CA-C-N	9.59	126.57	119.66
1	A	844	LEU	C-N-CA	9.59	126.57	119.66
1	C	613	LEU	CB-CA-C	8.52	127.38	110.42
1	A	613	LEU	CB-CA-C	8.51	127.36	110.42
1	B	613	LEU	CB-CA-C	8.51	127.36	110.42
1	C	337	PHE	CA-C-N	7.58	127.54	120.03
1	C	337	PHE	C-N-CA	7.58	127.54	120.03
1	B	337	PHE	CA-C-N	7.57	127.53	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	PHE	C-N-CA	7.57	127.53	120.03
1	B	845	PRO	CA-C-N	7.55	127.48	119.85
1	B	845	PRO	C-N-CA	7.55	127.48	119.85
1	A	337	PHE	CA-C-N	7.55	127.50	120.03
1	A	337	PHE	C-N-CA	7.55	127.50	120.03
1	C	845	PRO	CA-C-N	7.53	127.45	119.85
1	C	845	PRO	C-N-CA	7.53	127.45	119.85
1	A	845	PRO	CA-C-N	7.53	127.45	119.85
1	A	845	PRO	C-N-CA	7.53	127.45	119.85
1	B	1122	ASP	CA-C-N	7.21	126.88	119.82
1	B	1122	ASP	C-N-CA	7.21	126.88	119.82
1	C	1122	ASP	CA-C-N	7.21	126.88	119.82
1	C	1122	ASP	C-N-CA	7.21	126.88	119.82
1	A	1122	ASP	CA-C-N	7.20	126.87	119.82
1	A	1122	ASP	C-N-CA	7.20	126.87	119.82
1	C	924	THR	CA-C-N	7.09	126.79	119.56
1	C	924	THR	C-N-CA	7.09	126.79	119.56
1	B	1061	ALA	CA-C-N	7.07	126.70	119.56
1	B	1061	ALA	C-N-CA	7.07	126.70	119.56
1	C	1061	ALA	CA-C-N	7.07	126.70	119.56
1	C	1061	ALA	C-N-CA	7.07	126.70	119.56
1	A	1061	ALA	CA-C-N	7.05	126.68	119.56
1	A	1061	ALA	C-N-CA	7.05	126.68	119.56
1	B	924	THR	CA-C-N	7.04	126.75	119.56
1	B	924	THR	C-N-CA	7.04	126.75	119.56
1	C	794	LYS	CA-C-N	7.04	127.02	119.28
1	C	794	LYS	C-N-CA	7.04	127.02	119.28
1	A	924	THR	CA-C-N	7.03	126.73	119.56
1	A	924	THR	C-N-CA	7.03	126.73	119.56
1	A	794	LYS	CA-C-N	7.01	126.99	119.28
1	A	794	LYS	C-N-CA	7.01	126.99	119.28
1	C	799	SER	CA-C-N	7.01	126.53	119.24
1	C	799	SER	C-N-CA	7.01	126.53	119.24
1	A	799	SER	CA-C-N	7.00	126.52	119.24
1	A	799	SER	C-N-CA	7.00	126.52	119.24
1	B	794	LYS	CA-C-N	7.00	126.98	119.28
1	B	794	LYS	C-N-CA	7.00	126.98	119.28
1	B	799	SER	CA-C-N	6.99	126.51	119.24
1	B	799	SER	C-N-CA	6.99	126.51	119.24
1	A	27	LYS	CA-C-N	6.98	126.74	119.76
1	A	27	LYS	C-N-CA	6.98	126.74	119.76
1	B	84	ASN	CA-C-N	6.96	126.93	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ASN	C-N-CA	6.96	126.93	120.03
1	C	84	ASN	CA-C-N	6.96	126.92	120.03
1	C	84	ASN	C-N-CA	6.96	126.92	120.03
1	A	84	ASN	CA-C-N	6.95	126.91	120.03
1	A	84	ASN	C-N-CA	6.95	126.91	120.03
1	B	27	LYS	CA-C-N	6.95	126.71	119.76
1	B	27	LYS	C-N-CA	6.95	126.71	119.76
1	A	174	ASP	CA-C-N	6.94	127.50	120.14
1	A	174	ASP	C-N-CA	6.94	127.50	120.14
1	C	27	LYS	CA-C-N	6.93	126.69	119.76
1	C	27	LYS	C-N-CA	6.93	126.69	119.76
1	C	174	ASP	CA-C-N	6.93	127.49	120.14
1	C	174	ASP	C-N-CA	6.93	127.49	120.14
1	B	174	ASP	CA-C-N	6.93	127.48	120.14
1	B	174	ASP	C-N-CA	6.93	127.48	120.14
1	A	242	SER	CA-C-N	6.91	126.87	120.03
1	A	242	SER	C-N-CA	6.91	126.87	120.03
1	B	242	SER	CA-C-N	6.91	126.87	120.03
1	B	242	SER	C-N-CA	6.91	126.87	120.03
1	C	242	SER	CA-C-N	6.90	126.86	120.03
1	C	242	SER	C-N-CA	6.90	126.86	120.03
1	C	1094	SER	CA-C-N	6.89	127.14	119.90
1	C	1094	SER	C-N-CA	6.89	127.14	119.90
1	A	1094	SER	CA-C-N	6.87	127.11	119.90
1	A	1094	SER	C-N-CA	6.87	127.11	119.90
1	B	416	LEU	CA-C-N	6.85	126.81	120.03
1	B	416	LEU	C-N-CA	6.85	126.81	120.03
1	B	1094	SER	CA-C-N	6.84	127.08	119.90
1	B	1094	SER	C-N-CA	6.84	127.08	119.90
1	C	416	LEU	CA-C-N	6.84	126.80	120.03
1	C	416	LEU	C-N-CA	6.84	126.80	120.03
1	A	374	SER	CA-C-N	6.83	126.53	119.56
1	A	374	SER	C-N-CA	6.83	126.53	119.56
1	A	416	LEU	CA-C-N	6.82	126.78	120.03
1	A	416	LEU	C-N-CA	6.82	126.78	120.03
1	C	374	SER	CA-C-N	6.78	126.48	119.56
1	C	374	SER	C-N-CA	6.78	126.48	119.56
1	B	374	SER	CA-C-N	6.77	126.47	119.56
1	B	374	SER	C-N-CA	6.77	126.47	119.56
1	A	311	SER	CA-C-N	6.73	126.65	119.85
1	A	311	SER	C-N-CA	6.73	126.65	119.85
1	B	402	ALA	CA-C-N	6.72	126.71	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	ALA	C-N-CA	6.72	126.71	119.78
1	B	311	SER	CA-C-N	6.71	126.63	119.85
1	B	311	SER	C-N-CA	6.71	126.63	119.85
1	C	402	ALA	CA-C-N	6.70	126.68	119.78
1	C	402	ALA	C-N-CA	6.70	126.68	119.78
1	C	311	SER	CA-C-N	6.70	126.62	119.85
1	C	311	SER	C-N-CA	6.70	126.62	119.85
1	A	402	ALA	CA-C-N	6.70	126.68	119.78
1	A	402	ALA	C-N-CA	6.70	126.68	119.78
1	A	710	LEU	CA-C-N	6.67	126.64	119.76
1	A	710	LEU	C-N-CA	6.67	126.64	119.76
1	B	487	THR	CA-C-N	6.67	126.36	119.56
1	B	487	THR	C-N-CA	6.67	126.36	119.56
1	C	487	THR	CA-C-N	6.67	126.36	119.56
1	C	487	THR	C-N-CA	6.67	126.36	119.56
1	A	487	THR	CA-C-N	6.66	126.35	119.56
1	A	487	THR	C-N-CA	6.66	126.35	119.56
1	B	710	LEU	CA-C-N	6.65	126.61	119.76
1	B	710	LEU	C-N-CA	6.65	126.61	119.76
1	C	710	LEU	CA-C-N	6.64	126.60	119.76
1	C	710	LEU	C-N-CA	6.64	126.60	119.76
1	B	791	ASP	CA-C-N	6.58	126.72	119.87
1	B	791	ASP	C-N-CA	6.58	126.72	119.87
1	A	791	ASP	CA-C-N	6.58	126.71	119.87
1	A	791	ASP	C-N-CA	6.58	126.71	119.87
1	B	609	VAL	CA-C-N	6.57	126.26	119.82
1	B	609	VAL	C-N-CA	6.57	126.26	119.82
1	A	609	VAL	CA-C-N	6.56	126.25	119.82
1	A	609	VAL	C-N-CA	6.56	126.25	119.82
1	C	791	ASP	CA-C-N	6.56	126.69	119.87
1	C	791	ASP	C-N-CA	6.56	126.69	119.87
1	C	609	VAL	CA-C-N	6.56	126.25	119.82
1	C	609	VAL	C-N-CA	6.56	126.25	119.82
1	A	495	GLN	CA-C-N	6.48	126.24	119.76
1	A	495	GLN	C-N-CA	6.48	126.24	119.76
1	C	495	GLN	CA-C-N	6.46	126.22	119.76
1	C	495	GLN	C-N-CA	6.46	126.22	119.76
1	B	495	GLN	CA-C-N	6.46	126.22	119.76
1	B	495	GLN	C-N-CA	6.46	126.22	119.76
1	A	588	THR	CA-C-N	6.45	127.01	120.04
1	A	588	THR	C-N-CA	6.45	127.01	120.04
1	C	588	THR	CA-C-N	6.43	126.98	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	588	THR	C-N-CA	6.43	126.98	120.04
1	B	588	THR	CA-C-N	6.42	126.97	120.04
1	B	588	THR	C-N-CA	6.42	126.97	120.04
1	C	567	ASP	CA-C-N	6.41	127.85	119.84
1	C	567	ASP	C-N-CA	6.41	127.85	119.84
1	B	567	ASP	CA-C-N	6.40	127.84	119.84
1	B	567	ASP	C-N-CA	6.40	127.84	119.84
1	A	1051	VAL	CA-C-N	6.40	126.31	119.85
1	A	1051	VAL	C-N-CA	6.40	126.31	119.85
1	C	1051	VAL	CA-C-N	6.39	126.31	119.85
1	C	1051	VAL	C-N-CA	6.39	126.31	119.85
1	A	567	ASP	CA-C-N	6.38	127.82	119.84
1	A	567	ASP	C-N-CA	6.38	127.82	119.84
1	B	1051	VAL	CA-C-N	6.38	126.30	119.85
1	B	1051	VAL	C-N-CA	6.38	126.30	119.85
1	A	789	LEU	CA-C-N	6.35	126.27	119.85
1	A	789	LEU	C-N-CA	6.35	126.27	119.85
1	C	789	LEU	CA-C-N	6.33	126.24	119.85
1	C	789	LEU	C-N-CA	6.33	126.24	119.85
1	B	968	ASP	CA-C-N	6.33	126.89	120.38
1	B	968	ASP	C-N-CA	6.33	126.89	120.38
1	A	879	ILE	CA-C-N	6.32	126.27	119.76
1	A	879	ILE	C-N-CA	6.32	126.27	119.76
1	C	968	ASP	CA-C-N	6.32	126.89	120.38
1	C	968	ASP	C-N-CA	6.32	126.89	120.38
1	A	968	ASP	CA-C-N	6.31	126.88	120.38
1	A	968	ASP	C-N-CA	6.31	126.88	120.38
1	C	879	ILE	CA-C-N	6.31	126.26	119.76
1	C	879	ILE	C-N-CA	6.31	126.26	119.76
1	B	879	ILE	CA-C-N	6.31	126.26	119.76
1	B	879	ILE	C-N-CA	6.31	126.26	119.76
1	B	789	LEU	CA-C-N	6.30	126.22	119.85
1	B	789	LEU	C-N-CA	6.30	126.22	119.85
1	B	479	GLU	CA-C-N	6.22	126.12	119.28
1	B	479	GLU	C-N-CA	6.22	126.12	119.28
1	C	479	GLU	CA-C-N	6.22	126.12	119.28
1	C	479	GLU	C-N-CA	6.22	126.12	119.28
1	B	697	ILE	CA-C-N	6.20	126.15	119.76
1	B	697	ILE	C-N-CA	6.20	126.15	119.76
1	C	697	ILE	CA-C-N	6.20	126.14	119.76
1	C	697	ILE	C-N-CA	6.20	126.14	119.76
1	A	479	GLU	CA-C-N	6.18	126.08	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	GLU	C-N-CA	6.18	126.08	119.28
1	A	697	ILE	CA-C-N	6.17	126.11	119.76
1	A	697	ILE	C-N-CA	6.17	126.11	119.76
1	B	774	THR	CA-C-N	6.15	126.06	119.85
1	B	774	THR	C-N-CA	6.15	126.06	119.85
1	C	774	THR	CA-C-N	6.14	126.05	119.85
1	C	774	THR	C-N-CA	6.14	126.05	119.85
1	A	774	THR	CA-C-N	6.12	126.03	119.85
1	A	774	THR	C-N-CA	6.12	126.03	119.85
1	B	220	LYS	CA-C-N	6.12	125.88	119.76
1	B	220	LYS	C-N-CA	6.12	125.88	119.76
1	A	220	LYS	CA-C-N	6.11	125.87	119.76
1	A	220	LYS	C-N-CA	6.11	125.87	119.76
1	C	220	LYS	CA-C-N	6.11	125.87	119.76
1	C	220	LYS	C-N-CA	6.11	125.87	119.76
1	B	319	PHE	CA-C-N	6.06	126.03	120.03
1	B	319	PHE	C-N-CA	6.06	126.03	120.03
1	C	319	PHE	CA-C-N	6.06	126.03	120.03
1	C	319	PHE	C-N-CA	6.06	126.03	120.03
1	A	326	CYS	CA-C-N	6.04	127.39	119.84
1	A	326	CYS	C-N-CA	6.04	127.39	119.84
1	A	319	PHE	CA-C-N	6.04	126.01	120.03
1	A	319	PHE	C-N-CA	6.04	126.01	120.03
1	B	1035	PHE	CA-C-N	6.00	126.50	120.14
1	B	1035	PHE	C-N-CA	6.00	126.50	120.14
1	C	212	PHE	CA-C-N	5.99	126.34	119.93
1	C	212	PHE	C-N-CA	5.99	126.34	119.93
1	C	1035	PHE	CA-C-N	5.99	126.49	120.14
1	C	1035	PHE	C-N-CA	5.99	126.49	120.14
1	A	1035	PHE	CA-C-N	5.98	126.48	120.14
1	A	1035	PHE	C-N-CA	5.98	126.48	120.14
1	A	212	PHE	CA-C-N	5.97	126.32	119.93
1	A	212	PHE	C-N-CA	5.97	126.32	119.93
1	B	212	PHE	CA-C-N	5.97	126.32	119.93
1	B	212	PHE	C-N-CA	5.97	126.32	119.93
1	C	36	SER	CB-CA-C	-5.90	109.79	116.63
1	A	36	SER	CB-CA-C	-5.88	109.81	116.63
1	B	36	SER	CB-CA-C	-5.87	109.83	116.63
1	C	87	ILE	CA-C-N	5.77	125.78	119.90
1	C	87	ILE	C-N-CA	5.77	125.78	119.90
1	A	87	ILE	CA-C-N	5.75	125.77	119.90
1	A	87	ILE	C-N-CA	5.75	125.77	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ILE	CA-C-N	5.75	125.76	119.90
1	B	87	ILE	C-N-CA	5.75	125.76	119.90
1	B	60	LEU	CA-C-N	5.68	125.63	119.78
1	B	60	LEU	C-N-CA	5.68	125.63	119.78
1	C	60	LEU	CA-C-N	5.68	125.63	119.78
1	C	60	LEU	C-N-CA	5.68	125.63	119.78
1	A	60	LEU	CA-C-N	5.67	125.62	119.78
1	A	60	LEU	C-N-CA	5.67	125.62	119.78
1	C	1072	PHE	CA-C-N	5.66	125.42	119.76
1	C	1072	PHE	C-N-CA	5.66	125.42	119.76
1	B	1072	PHE	CA-C-N	5.65	125.41	119.76
1	B	1072	PHE	C-N-CA	5.65	125.41	119.76
1	A	1072	PHE	CA-C-N	5.64	125.40	119.76
1	A	1072	PHE	C-N-CA	5.64	125.40	119.76
1	C	549	GLN	CA-C-N	5.58	125.68	119.32
1	C	549	GLN	C-N-CA	5.58	125.68	119.32
1	B	549	GLN	CA-C-N	5.58	125.68	119.32
1	B	549	GLN	C-N-CA	5.58	125.68	119.32
1	A	549	GLN	CA-C-N	5.56	125.66	119.32
1	A	549	GLN	C-N-CA	5.56	125.66	119.32
1	A	509	ALA	CA-C-N	5.55	125.86	119.93
1	A	509	ALA	C-N-CA	5.55	125.86	119.93
1	B	509	ALA	CA-C-N	5.54	125.86	119.93
1	B	509	ALA	C-N-CA	5.54	125.86	119.93
1	C	509	ALA	CA-C-N	5.52	125.84	119.93
1	C	509	ALA	C-N-CA	5.52	125.84	119.93
1	A	655	ILE	CA-C-N	5.44	125.20	119.76
1	A	655	ILE	C-N-CA	5.44	125.20	119.76
1	B	655	ILE	CA-C-N	5.40	125.16	119.76
1	B	655	ILE	C-N-CA	5.40	125.16	119.76
1	C	655	ILE	CA-C-N	5.39	125.15	119.76
1	C	655	ILE	C-N-CA	5.39	125.15	119.76
1	A	451	LYS	CA-C-N	5.33	125.64	119.93
1	A	451	LYS	C-N-CA	5.33	125.64	119.93
1	B	451	LYS	CA-C-N	5.33	125.63	119.93
1	B	451	LYS	C-N-CA	5.33	125.63	119.93
1	C	451	LYS	CA-C-N	5.32	125.62	119.93
1	C	451	LYS	C-N-CA	5.32	125.62	119.93
1	B	261	LYS	CA-C-N	5.29	126.46	119.84
1	B	261	LYS	C-N-CA	5.29	126.46	119.84
1	B	141	ASP	CA-C-N	5.29	125.54	119.83
1	B	141	ASP	C-N-CA	5.29	125.54	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	261	LYS	CA-C-N	5.28	126.44	119.84
1	C	261	LYS	C-N-CA	5.28	126.44	119.84
1	A	261	LYS	CA-C-N	5.28	126.44	119.84
1	A	261	LYS	C-N-CA	5.28	126.44	119.84
1	C	141	ASP	CA-C-N	5.25	125.50	119.83
1	C	141	ASP	C-N-CA	5.25	125.50	119.83
1	A	141	ASP	CA-C-N	5.23	125.48	119.83
1	A	141	ASP	C-N-CA	5.23	125.48	119.83
1	C	874	GLY	N-CA-C	-5.13	108.59	115.32
1	B	874	GLY	N-CA-C	-5.13	108.60	115.32
1	A	874	GLY	N-CA-C	-5.12	108.62	115.32
1	A	881	PHE	CA-C-N	5.02	125.30	119.47
1	A	881	PHE	C-N-CA	5.02	125.30	119.47
1	C	881	PHE	CA-C-N	5.01	125.29	119.47
1	C	881	PHE	C-N-CA	5.01	125.29	119.47

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	8073	0	7497	26	0
1	B	8075	0	7502	28	0
1	C	8078	0	7504	28	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	W	28	0	25	0	0
2	X	28	0	25	0	0
2	Y	28	0	25	0	0
2	Z	28	0	25	0	0
2	c	28	0	25	0	0
2	d	28	0	25	0	0
2	e	28	0	25	0	0
2	f	28	0	25	0	0
2	g	28	0	25	0	0
3	G	50	0	43	0	0
3	Q	50	0	43	0	0
3	a	50	0	43	0	0
4	H	72	0	61	0	0
4	R	72	0	61	0	0
4	b	72	0	61	0	0
5	A	154	0	143	3	0
5	B	154	0	143	3	0
5	C	154	0	143	2	0
All	All	25726	0	23844	79	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 2.

All (79) 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:767:GLN:HG3	1:C:1012:MET:HG2	1.63	0.81
1:B:767:GLN:HG3	1:B:1012:MET:HG2	1.63	0.80
1:A:767:GLN:HG3	1:A:1012:MET:HG2	1.63	0.79
1:A:767:GLN:HG3	1:A:1012:MET:CG	2.23	0.68
1:B:767:GLN:HG3	1:B:1012:MET:CG	2.23	0.68
1:C:767:GLN:HG3	1:C:1012:MET:CG	2.23	0.68
1:B:1069:LYS:HD3	1:B:1105:GLU:OE2	2.02	0.60
1:C:1069:LYS:HD3	1:C:1105:GLU:OE2	2.02	0.60
1:C:319:PHE:O	1:C:569:LYS:HE3	2.02	0.60
1:A:319:PHE:O	1:A:569:LYS:HE3	2.02	0.59
1:A:1069:LYS:HD3	1:A:1105:GLU:OE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:PHE:O	1:B:569:LYS:HE3	2.02	0.59
1:C:609:VAL:N	1:C:610:PRO:CD	2.69	0.55
1:A:609:VAL:N	1:A:610:PRO:CD	2.69	0.55
1:B:609:VAL:N	1:B:610:PRO:CD	2.69	0.55
1:C:347:ARG:HH22	1:C:385:SER:HA	1.74	0.53
1:B:347:ARG:HH22	1:B:385:SER:HA	1.74	0.52
1:A:347:ARG:HH22	1:A:385:SER:HA	1.74	0.51
1:B:519:SER:HB2	1:B:569:LYS:NZ	2.26	0.51
1:A:519:SER:HB2	1:A:569:LYS:NZ	2.26	0.51
1:C:519:SER:HB2	1:C:569:LYS:NZ	2.26	0.50
1:B:519:SER:CB	1:B:569:LYS:HZ2	2.25	0.49
1:B:881:PHE:N	1:B:882:PRO:CD	2.76	0.49
5:A:1305:NAG:H82	1:C:445:PHE:CE2	2.49	0.48
1:A:881:PHE:N	1:A:882:PRO:CD	2.76	0.48
1:C:881:PHE:N	1:C:882:PRO:CD	2.76	0.48
1:B:519:SER:HB2	1:B:569:LYS:HZ2	1.78	0.48
1:A:445:PHE:CE2	5:B:1305:NAG:H82	2.49	0.47
1:B:445:PHE:CE2	5:C:1305:NAG:H82	2.49	0.47
1:B:84:ASN:N	1:B:85:PRO:CD	2.79	0.45
1:C:84:ASN:N	1:C:85:PRO:CD	2.79	0.45
1:B:891:GLY:O	1:B:1021:LYS:NZ	2.49	0.45
1:A:891:GLY:O	1:A:1021:LYS:NZ	2.49	0.45
5:A:1305:NAG:H83	1:C:478:TYR:CE1	2.52	0.45
1:C:891:GLY:O	1:C:1021:LYS:NZ	2.49	0.45
1:A:84:ASN:N	1:A:85:PRO:CD	2.79	0.45
1:B:478:TYR:CE1	5:C:1305:NAG:H83	2.52	0.45
1:B:25:LYS:HD2	1:B:82:PHE:HB3	1.99	0.44
1:C:243:PRO:C	1:C:245:THR:H	2.26	0.44
1:A:478:TYR:CE1	5:B:1305:NAG:H83	2.52	0.44
1:A:25:LYS:HD2	1:A:82:PHE:HB3	1.99	0.44
1:C:25:LYS:HD2	1:C:82:PHE:HB3	1.99	0.44
1:A:683:GLY:HA3	1:B:769:LYS:O	2.18	0.44
1:B:683:GLY:HA3	1:C:769:LYS:O	2.18	0.44
1:B:243:PRO:C	1:B:245:THR:H	2.26	0.44
1:A:243:PRO:C	1:A:245:THR:H	2.26	0.43
1:B:270:ASP:OD1	1:B:270:ASP:C	2.62	0.43
1:C:270:ASP:OD1	1:C:270:ASP:C	2.62	0.43
1:A:270:ASP:OD1	1:A:270:ASP:C	2.62	0.43
1:A:769:LYS:O	1:C:683:GLY:HA3	2.18	0.43
1:B:408:VAL:HG23	1:B:409:ILE:N	2.34	0.43
1:A:989:THR:O	1:A:993:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ASN:O	1:B:179:THR:C	2.62	0.42
1:B:989:THR:O	1:B:993:GLN:HG3	2.19	0.42
1:C:178:ASN:O	1:C:179:THR:C	2.62	0.42
1:A:44:ASP:OD1	1:A:45:ASP:N	2.53	0.42
1:A:408:VAL:HG23	1:A:409:ILE:N	2.34	0.42
1:B:44:ASP:OD1	1:B:45:ASP:N	2.53	0.42
1:C:44:ASP:OD1	1:C:45:ASP:N	2.53	0.42
1:C:989:THR:O	1:C:993:GLN:HG3	2.19	0.42
1:A:178:ASN:O	1:A:179:THR:C	2.62	0.41
1:B:84:ASN:N	1:B:85:PRO:HD3	2.35	0.41
1:A:84:ASN:N	1:A:85:PRO:HD3	2.35	0.41
1:A:519:SER:CB	1:A:569:LYS:NZ	2.83	0.41
1:C:408:VAL:HG23	1:C:409:ILE:N	2.34	0.41
1:C:531:ASN:OD1	1:C:531:ASN:C	2.63	0.41
1:C:519:SER:CB	1:C:569:LYS:NZ	2.83	0.41
1:B:779:ASP:OD1	1:B:779:ASP:C	2.64	0.41
1:C:84:ASN:N	1:C:85:PRO:HD3	2.35	0.41
1:A:531:ASN:OD1	1:A:531:ASN:C	2.63	0.41
1:B:531:ASN:OD1	1:B:531:ASN:C	2.63	0.41
1:B:881:PHE:HB3	1:B:882:PRO:HD3	2.03	0.41
1:A:969:PRO:N	1:A:970:PRO:CD	2.83	0.41
1:C:519:SER:CB	1:C:569:LYS:HZ2	2.34	0.40
1:C:767:GLN:CG	1:C:1012:MET:HG2	2.43	0.40
1:A:478:TYR:CZ	5:B:1305:NAG:H83	2.57	0.40
1:C:969:PRO:N	1:C:970:PRO:CD	2.83	0.40
5:A:1305:NAG:H83	1:C:478:TYR:CZ	2.57	0.40
1:B:969:PRO:N	1:B:970:PRO:CD	2.83	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	1076/1280 (84%)	1027 (95%)	47 (4%)	2 (0%)	43	72
1	B	1076/1280 (84%)	1027 (95%)	47 (4%)	2 (0%)	43	72
1	C	1076/1280 (84%)	1027 (95%)	47 (4%)	2 (0%)	43	72
All	All	3228/3840 (84%)	3081 (95%)	141 (4%)	6 (0%)	44	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	614	HIS
1	B	614	HIS
1	C	614	HIS
1	A	179	THR
1	B	179	THR
1	C	179	THR

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	798/1108 (72%)	789 (99%)	9 (1%)	65	87
1	B	799/1108 (72%)	790 (99%)	9 (1%)	65	87
1	C	800/1108 (72%)	791 (99%)	9 (1%)	65	87
All	All	2397/3324 (72%)	2370 (99%)	27 (1%)	63	87

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	148	ASN
1	A	360	ASN
1	A	526	LYS
1	A	547	LYS
1	A	592	ASN
1	A	905	GLN

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Mol	Chain	Res	Type
1	A	1055	GLN
1	A	1117	ASN
1	B	125	ASN
1	B	148	ASN
1	B	360	ASN
1	B	526	LYS
1	B	547	LYS
1	B	592	ASN
1	B	905	GLN
1	B	1055	GLN
1	B	1117	ASN
1	C	125	ASN
1	C	148	ASN
1	C	360	ASN
1	C	526	LYS
1	C	547	LYS
1	C	592	ASN
1	C	905	GLN
1	C	1055	GLN
1	C	1117	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	HIS
1	A	188	HIS
1	A	890	ASN
1	A	918	GLN
1	A	988	GLN
1	A	1055	GLN
1	A	1084	HIS
1	B	184	HIS
1	B	188	HIS
1	B	747	ASN
1	B	890	ASN
1	B	918	GLN
1	B	988	GLN
1	B	1055	GLN
1	B	1084	HIS
1	C	184	HIS
1	C	188	HIS
1	C	890	ASN

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Mol	Chain	Res	Type
1	C	918	GLN
1	C	988	GLN
1	C	1055	GLN
1	C	1084	HIS

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 ⓘ

78 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	1,2	14,14,15	1.31	1 (7%)	17,19,21	1.08	1 (5%)
2	NAG	D	2	2	14,14,15	1.18	1 (7%)	17,19,21	0.96	1 (5%)
2	NAG	E	1	1,2	14,14,15	1.41	1 (7%)	17,19,21	1.01	1 (5%)
2	NAG	E	2	2	14,14,15	1.12	1 (7%)	17,19,21	0.88	1 (5%)
2	NAG	F	1	1,2	14,14,15	1.39	2 (14%)	17,19,21	1.04	1 (5%)
2	NAG	F	2	2	14,14,15	1.17	1 (7%)	17,19,21	0.95	1 (5%)
3	NAG	G	1	1,3	14,14,15	1.20	2 (14%)	17,19,21	1.23	2 (11%)
3	NAG	G	2	3	14,14,15	1.25	1 (7%)	17,19,21	1.06	1 (5%)
3	BMA	G	3	3	11,11,12	0.66	0	15,15,17	0.87	0
3	MAN	G	4	3	11,11,12	1.01	0	15,15,17	0.49	0
4	NAG	H	1	1,4	14,14,15	1.25	1 (7%)	17,19,21	1.16	2 (11%)
4	NAG	H	2	4	14,14,15	1.17	2 (14%)	17,19,21	1.03	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	H	3	4	11,11,12	1.28	1 (9%)	15,15,17	0.78	0
4	MAN	H	4	4	11,11,12	0.61	0	15,15,17	0.66	0
4	MAN	H	5	4	11,11,12	0.95	0	15,15,17	0.74	1 (6%)
4	MAN	H	6	4	11,11,12	1.16	1 (9%)	15,15,17	0.89	1 (6%)
2	NAG	I	1	1,2	14,14,15	1.25	1 (7%)	17,19,21	0.92	1 (5%)
2	NAG	I	2	2	14,14,15	1.22	1 (7%)	17,19,21	0.93	1 (5%)
2	NAG	J	1	1,2	14,14,15	1.30	1 (7%)	17,19,21	1.07	2 (11%)
2	NAG	J	2	2	14,14,15	1.14	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	K	1	1,2	14,14,15	1.27	1 (7%)	17,19,21	1.07	1 (5%)
2	NAG	K	2	2	14,14,15	1.20	1 (7%)	17,19,21	0.96	1 (5%)
2	NAG	L	1	1,2	14,14,15	1.28	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	L	2	2	14,14,15	1.18	1 (7%)	17,19,21	0.94	1 (5%)
2	NAG	M	1	1,2	14,14,15	1.35	1 (7%)	17,19,21	1.13	2 (11%)
2	NAG	M	2	2	14,14,15	1.15	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	N	1	1,2	14,14,15	1.31	1 (7%)	17,19,21	1.08	1 (5%)
2	NAG	N	2	2	14,14,15	1.17	1 (7%)	17,19,21	0.96	1 (5%)
2	NAG	O	1	1,2	14,14,15	1.41	1 (7%)	17,19,21	1.01	1 (5%)
2	NAG	O	2	2	14,14,15	1.12	1 (7%)	17,19,21	0.89	1 (5%)
2	NAG	P	1	1,2	14,14,15	1.38	2 (14%)	17,19,21	1.04	1 (5%)
2	NAG	P	2	2	14,14,15	1.17	1 (7%)	17,19,21	0.95	1 (5%)
3	NAG	Q	1	1,3	14,14,15	1.19	2 (14%)	17,19,21	1.23	2 (11%)
3	NAG	Q	2	3	14,14,15	1.24	1 (7%)	17,19,21	1.06	1 (5%)
3	BMA	Q	3	3	11,11,12	0.66	0	15,15,17	0.87	0
3	MAN	Q	4	3	11,11,12	1.00	0	15,15,17	0.49	0
4	NAG	R	1	1,4	14,14,15	1.25	1 (7%)	17,19,21	1.16	2 (11%)
4	NAG	R	2	4	14,14,15	1.19	2 (14%)	17,19,21	1.03	1 (5%)
4	BMA	R	3	4	11,11,12	1.29	1 (9%)	15,15,17	0.79	0
4	MAN	R	4	4	11,11,12	0.60	0	15,15,17	0.66	0
4	MAN	R	5	4	11,11,12	0.95	0	15,15,17	0.74	1 (6%)
4	MAN	R	6	4	11,11,12	1.16	1 (9%)	15,15,17	0.89	1 (6%)
2	NAG	S	1	1,2	14,14,15	1.26	1 (7%)	17,19,21	0.92	1 (5%)
2	NAG	S	2	2	14,14,15	1.22	1 (7%)	17,19,21	0.92	1 (5%)
2	NAG	T	1	1,2	14,14,15	1.31	1 (7%)	17,19,21	1.08	2 (11%)
2	NAG	T	2	2	14,14,15	1.14	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	U	1	1,2	14,14,15	1.28	1 (7%)	17,19,21	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	U	2	2	14,14,15	1.21	1 (7%)	17,19,21	0.96	1 (5%)
2	NAG	V	1	1,2	14,14,15	1.28	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	V	2	2	14,14,15	1.17	1 (7%)	17,19,21	0.95	1 (5%)
2	NAG	W	1	1,2	14,14,15	1.35	1 (7%)	17,19,21	1.13	2 (11%)
2	NAG	W	2	2	14,14,15	1.15	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	X	1	1,2	14,14,15	1.31	1 (7%)	17,19,21	1.08	1 (5%)
2	NAG	X	2	2	14,14,15	1.17	1 (7%)	17,19,21	0.96	1 (5%)
2	NAG	Y	1	1,2	14,14,15	1.41	1 (7%)	17,19,21	1.01	1 (5%)
2	NAG	Y	2	2	14,14,15	1.11	1 (7%)	17,19,21	0.89	1 (5%)
2	NAG	Z	1	1,2	14,14,15	1.38	2 (14%)	17,19,21	1.04	1 (5%)
2	NAG	Z	2	2	14,14,15	1.17	1 (7%)	17,19,21	0.96	1 (5%)
3	NAG	a	1	1,3	14,14,15	1.20	2 (14%)	17,19,21	1.23	2 (11%)
3	NAG	a	2	3	14,14,15	1.25	1 (7%)	17,19,21	1.06	1 (5%)
3	BMA	a	3	3	11,11,12	0.66	0	15,15,17	0.87	0
3	MAN	a	4	3	11,11,12	1.02	0	15,15,17	0.49	0
4	NAG	b	1	1,4	14,14,15	1.26	1 (7%)	17,19,21	1.16	2 (11%)
4	NAG	b	2	4	14,14,15	1.18	2 (14%)	17,19,21	1.03	1 (5%)
4	BMA	b	3	4	11,11,12	1.29	1 (9%)	15,15,17	0.78	0
4	MAN	b	4	4	11,11,12	0.60	0	15,15,17	0.66	0
4	MAN	b	5	4	11,11,12	0.95	0	15,15,17	0.74	1 (6%)
4	MAN	b	6	4	11,11,12	1.15	1 (9%)	15,15,17	0.88	1 (6%)
2	NAG	c	1	1,2	14,14,15	1.26	1 (7%)	17,19,21	0.92	1 (5%)
2	NAG	c	2	2	14,14,15	1.22	1 (7%)	17,19,21	0.93	1 (5%)
2	NAG	d	1	1,2	14,14,15	1.31	1 (7%)	17,19,21	1.08	2 (11%)
2	NAG	d	2	2	14,14,15	1.13	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	e	1	1,2	14,14,15	1.28	2 (14%)	17,19,21	1.08	1 (5%)
2	NAG	e	2	2	14,14,15	1.21	1 (7%)	17,19,21	0.96	1 (5%)
2	NAG	f	1	1,2	14,14,15	1.28	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	f	2	2	14,14,15	1.18	1 (7%)	17,19,21	0.95	1 (5%)
2	NAG	g	1	1,2	14,14,15	1.35	1 (7%)	17,19,21	1.13	2 (11%)
2	NAG	g	2	2	14,14,15	1.15	1 (7%)	17,19,21	1.04	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
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	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	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	MAN	G	4	3	-	1/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	2/2/19/22	0/1/1/1
4	MAN	H	5	4	-	2/2/19/22	0/1/1/1
4	MAN	H	6	4	-	0/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	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	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	1/2/19/22	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	BMA	R	3	4	-	0/2/19/22	0/1/1/1
4	MAN	R	4	4	-	2/2/19/22	0/1/1/1

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

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C1-C2	4.07	1.57	1.52
2	P	1	NAG	C1-C2	4.07	1.57	1.52
2	W	1	NAG	C1-C2	4.06	1.57	1.52
2	M	1	NAG	C1-C2	4.05	1.57	1.52
2	g	1	NAG	C1-C2	4.05	1.57	1.52
2	Z	1	NAG	C1-C2	4.03	1.57	1.52
2	Y	1	NAG	C1-C2	4.03	1.57	1.52
2	O	1	NAG	C1-C2	4.02	1.57	1.52
2	E	1	NAG	C1-C2	4.02	1.57	1.52
2	N	1	NAG	C1-C2	3.91	1.57	1.52
2	X	1	NAG	C1-C2	3.91	1.57	1.52
2	D	1	NAG	C1-C2	3.89	1.57	1.52
4	b	1	NAG	C1-C2	3.88	1.57	1.52
2	d	1	NAG	C1-C2	3.87	1.57	1.52
2	T	1	NAG	C1-C2	3.87	1.57	1.52
2	J	1	NAG	C1-C2	3.84	1.57	1.52
4	R	1	NAG	C1-C2	3.82	1.57	1.52
4	H	1	NAG	C1-C2	3.82	1.57	1.52
2	f	1	NAG	C1-C2	3.80	1.57	1.52
2	V	1	NAG	C1-C2	3.80	1.57	1.52
2	L	1	NAG	C1-C2	3.78	1.57	1.52
2	e	1	NAG	C1-C2	3.75	1.57	1.52
2	U	1	NAG	C1-C2	3.74	1.57	1.52
2	K	1	NAG	C1-C2	3.73	1.57	1.52
2	S	1	NAG	C1-C2	3.68	1.57	1.52
2	I	2	NAG	C1-C2	3.68	1.57	1.52
2	c	1	NAG	C1-C2	3.66	1.57	1.52
2	c	2	NAG	C1-C2	3.65	1.57	1.52
2	S	2	NAG	C1-C2	3.65	1.57	1.52
2	I	1	NAG	C1-C2	3.64	1.57	1.52
2	e	2	NAG	C1-C2	3.57	1.57	1.52
3	G	2	NAG	C1-C2	3.56	1.57	1.52
3	a	2	NAG	C1-C2	3.55	1.57	1.52
2	U	2	NAG	C1-C2	3.55	1.57	1.52
3	Q	2	NAG	C1-C2	3.54	1.57	1.52
2	K	2	NAG	C1-C2	3.53	1.57	1.52
2	D	2	NAG	C1-C2	3.51	1.57	1.52
2	X	2	NAG	C1-C2	3.50	1.57	1.52
2	N	2	NAG	C1-C2	3.48	1.57	1.52
2	L	2	NAG	C1-C2	3.47	1.57	1.52
2	f	2	NAG	C1-C2	3.46	1.57	1.52
2	V	2	NAG	C1-C2	3.45	1.57	1.52
2	M	2	NAG	C1-C2	3.37	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	g	2	NAG	C1-C2	3.37	1.56	1.52
2	J	2	NAG	C1-C2	3.37	1.56	1.52
2	W	2	NAG	C1-C2	3.36	1.56	1.52
2	T	2	NAG	C1-C2	3.34	1.56	1.52
2	d	2	NAG	C1-C2	3.34	1.56	1.52
4	R	2	NAG	C1-C2	3.31	1.56	1.52
3	G	1	NAG	C1-C2	3.31	1.56	1.52
3	a	1	NAG	C1-C2	3.31	1.56	1.52
2	P	2	NAG	C1-C2	3.28	1.56	1.52
3	Q	1	NAG	C1-C2	3.28	1.56	1.52
4	b	2	NAG	C1-C2	3.26	1.56	1.52
2	Z	2	NAG	C1-C2	3.26	1.56	1.52
2	F	2	NAG	C1-C2	3.25	1.56	1.52
4	H	2	NAG	C1-C2	3.23	1.56	1.52
2	O	2	NAG	C1-C2	2.92	1.56	1.52
2	E	2	NAG	C1-C2	2.91	1.56	1.52
2	Y	2	NAG	C1-C2	2.89	1.56	1.52
4	H	3	BMA	O5-C5	2.57	1.48	1.43
4	R	3	BMA	O5-C5	2.57	1.48	1.43
4	b	3	BMA	O5-C5	2.55	1.48	1.43
4	H	6	MAN	C2-C3	2.34	1.56	1.52
4	R	6	MAN	C2-C3	2.33	1.56	1.52
4	b	6	MAN	C2-C3	2.29	1.56	1.52
2	P	1	NAG	O5-C5	2.06	1.47	1.43
2	Z	1	NAG	O5-C5	2.05	1.47	1.43
4	R	2	NAG	O5-C5	2.05	1.47	1.43
2	F	1	NAG	O5-C5	2.04	1.47	1.43
3	a	1	NAG	O5-C5	2.03	1.47	1.43
3	G	1	NAG	O5-C5	2.03	1.47	1.43
4	b	2	NAG	O5-C5	2.03	1.47	1.43
4	H	2	NAG	O5-C5	2.02	1.47	1.43
3	Q	1	NAG	O5-C5	2.02	1.47	1.43
2	e	1	NAG	O5-C5	2.00	1.47	1.43

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C8-C7-N2	2.98	121.05	116.12
3	a	1	NAG	C8-C7-N2	2.96	121.03	116.12
3	Q	1	NAG	C8-C7-N2	2.96	121.03	116.12
4	H	1	NAG	C8-C7-N2	2.87	120.88	116.12
4	R	1	NAG	C8-C7-N2	2.86	120.87	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	b	1	NAG	C8-C7-N2	2.86	120.86	116.12
2	U	1	NAG	C8-C7-N2	2.80	120.77	116.12
2	e	1	NAG	C8-C7-N2	2.80	120.76	116.12
4	H	2	NAG	C8-C7-N2	2.79	120.75	116.12
4	b	2	NAG	C8-C7-N2	2.79	120.74	116.12
2	K	1	NAG	C8-C7-N2	2.79	120.74	116.12
4	R	2	NAG	C8-C7-N2	2.78	120.73	116.12
2	g	2	NAG	C8-C7-N2	2.70	120.59	116.12
2	M	2	NAG	C8-C7-N2	2.69	120.58	116.12
2	W	2	NAG	C8-C7-N2	2.69	120.57	116.12
2	T	2	NAG	C8-C7-N2	2.66	120.53	116.12
2	J	2	NAG	C8-C7-N2	2.65	120.52	116.12
2	d	2	NAG	C8-C7-N2	2.65	120.51	116.12
2	X	1	NAG	C8-C7-N2	2.62	120.46	116.12
2	E	1	NAG	C8-C7-N2	2.61	120.45	116.12
2	D	1	NAG	C8-C7-N2	2.61	120.45	116.12
2	N	1	NAG	C8-C7-N2	2.61	120.44	116.12
2	O	1	NAG	C8-C7-N2	2.60	120.44	116.12
2	Z	1	NAG	C8-C7-N2	2.59	120.42	116.12
2	Y	1	NAG	C8-C7-N2	2.59	120.41	116.12
2	F	1	NAG	C8-C7-N2	2.59	120.41	116.12
2	P	1	NAG	C8-C7-N2	2.58	120.40	116.12
2	g	1	NAG	C8-C7-N2	2.56	120.36	116.12
2	M	1	NAG	C8-C7-N2	2.55	120.36	116.12
2	W	1	NAG	C8-C7-N2	2.55	120.34	116.12
2	S	2	NAG	C8-C7-N2	2.52	120.30	116.12
2	I	2	NAG	C8-C7-N2	2.52	120.29	116.12
2	c	2	NAG	C8-C7-N2	2.51	120.29	116.12
2	X	2	NAG	C8-C7-N2	2.51	120.28	116.12
2	N	2	NAG	C8-C7-N2	2.51	120.28	116.12
2	f	1	NAG	C8-C7-N2	2.51	120.28	116.12
2	D	2	NAG	C8-C7-N2	2.51	120.27	116.12
2	V	1	NAG	C8-C7-N2	2.50	120.27	116.12
2	L	1	NAG	C8-C7-N2	2.50	120.26	116.12
3	a	2	NAG	C8-C7-N2	2.47	120.22	116.12
3	Q	2	NAG	C8-C7-N2	2.47	120.21	116.12
3	G	2	NAG	C8-C7-N2	2.47	120.21	116.12
2	d	1	NAG	C1-C2-N2	-2.39	106.67	110.43
2	T	1	NAG	C1-C2-N2	-2.38	106.68	110.43
2	K	2	NAG	C8-C7-N2	2.36	120.03	116.12
2	f	2	NAG	C8-C7-N2	2.36	120.03	116.12
2	J	1	NAG	C1-C2-N2	-2.36	106.72	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	2	NAG	C8-C7-N2	2.35	120.02	116.12
2	e	2	NAG	C8-C7-N2	2.35	120.01	116.12
2	V	2	NAG	C8-C7-N2	2.35	120.01	116.12
2	L	2	NAG	C8-C7-N2	2.34	120.00	116.12
2	I	1	NAG	C8-C7-N2	2.24	119.84	116.12
2	O	2	NAG	C8-C7-N2	2.24	119.84	116.12
4	b	5	MAN	C1-C2-C3	-2.24	106.38	109.64
2	c	1	NAG	C8-C7-N2	2.24	119.83	116.12
2	S	1	NAG	C8-C7-N2	2.24	119.83	116.12
2	E	2	NAG	C8-C7-N2	2.23	119.82	116.12
4	H	5	MAN	C1-C2-C3	-2.23	106.39	109.64
2	Y	2	NAG	C8-C7-N2	2.23	119.81	116.12
4	R	5	MAN	C1-C2-C3	-2.22	106.41	109.64
2	Z	2	NAG	C8-C7-N2	2.22	119.79	116.12
2	P	2	NAG	C8-C7-N2	2.22	119.79	116.12
2	F	2	NAG	C8-C7-N2	2.21	119.78	116.12
2	W	1	NAG	C2-N2-C7	-2.20	119.95	122.90
4	R	6	MAN	C2-C3-C4	-2.19	107.00	110.86
2	M	1	NAG	C2-N2-C7	-2.19	119.96	122.90
2	g	1	NAG	C2-N2-C7	-2.19	119.96	122.90
4	H	6	MAN	C2-C3-C4	-2.18	107.02	110.86
4	b	6	MAN	C2-C3-C4	-2.17	107.05	110.86
2	T	1	NAG	C8-C7-N2	2.16	119.69	116.12
2	J	1	NAG	C8-C7-N2	2.14	119.67	116.12
2	d	1	NAG	C8-C7-N2	2.14	119.66	116.12
4	b	1	NAG	C2-N2-C7	-2.08	120.12	122.90
4	H	1	NAG	C2-N2-C7	-2.06	120.14	122.90
4	R	1	NAG	C2-N2-C7	-2.05	120.15	122.90
3	Q	1	NAG	C2-N2-C7	-2.04	120.16	122.90
3	G	1	NAG	C2-N2-C7	-2.03	120.17	122.90
3	a	1	NAG	C2-N2-C7	-2.03	120.19	122.90

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	4	MAN	O5-C5-C6-O6
4	H	5	MAN	O5-C5-C6-O6
4	R	4	MAN	O5-C5-C6-O6
4	R	5	MAN	O5-C5-C6-O6
4	b	4	MAN	O5-C5-C6-O6
4	b	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	G	3	BMA	O5-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
3	a	3	BMA	O5-C5-C6-O6
4	H	5	MAN	C4-C5-C6-O6
4	R	5	MAN	C4-C5-C6-O6
4	b	5	MAN	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	a	3	BMA	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	Q	3	BMA	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
4	H	4	MAN	C4-C5-C6-O6
4	R	4	MAN	C4-C5-C6-O6
4	b	4	MAN	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	c	1	NAG	C4-C5-C6-O6
2	U	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	e	2	NAG	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	e	2	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	c	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	c	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
3	G	4	MAN	C4-C5-C6-O6
3	Q	4	MAN	C4-C5-C6-O6
3	a	4	MAN	C4-C5-C6-O6

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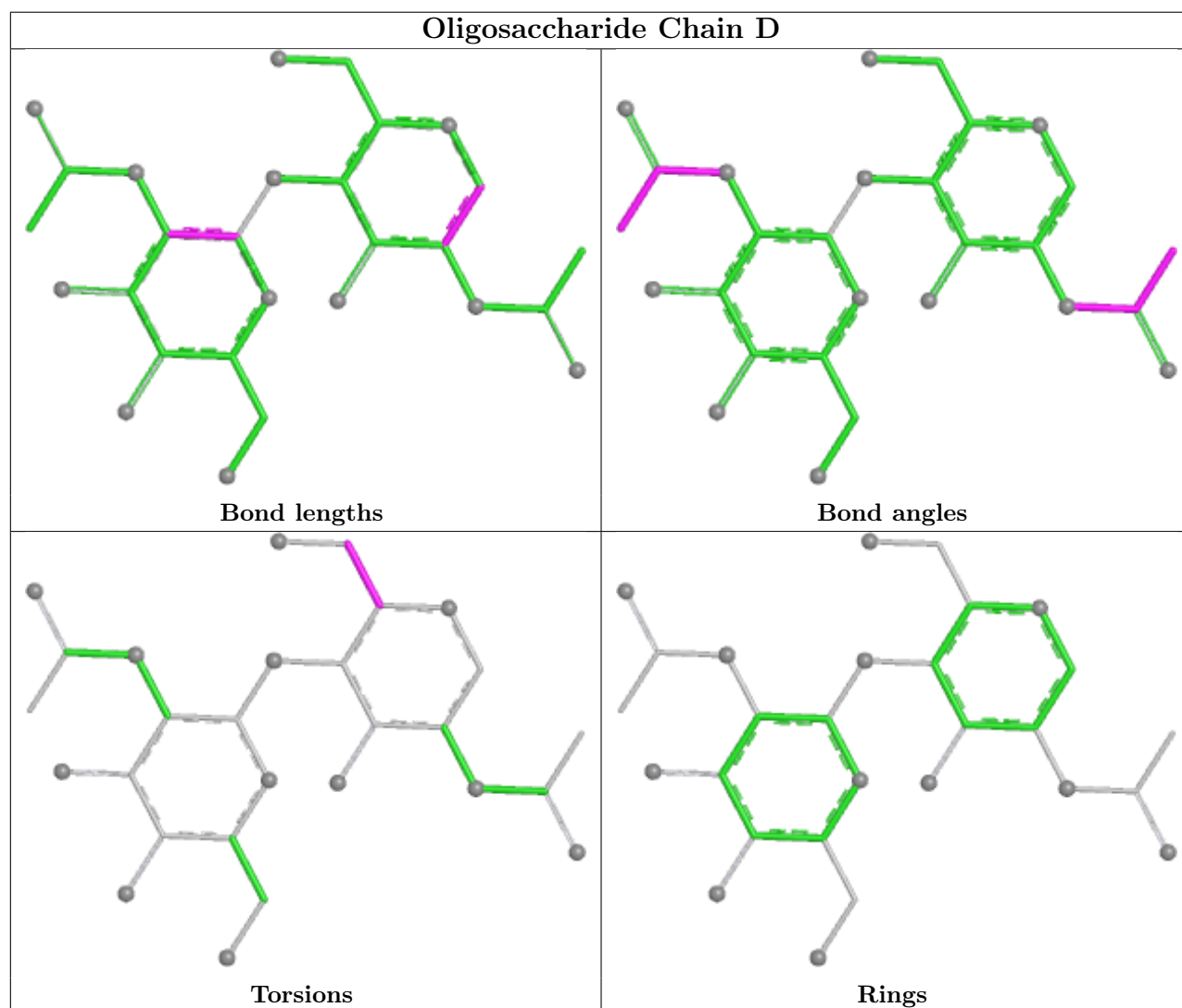
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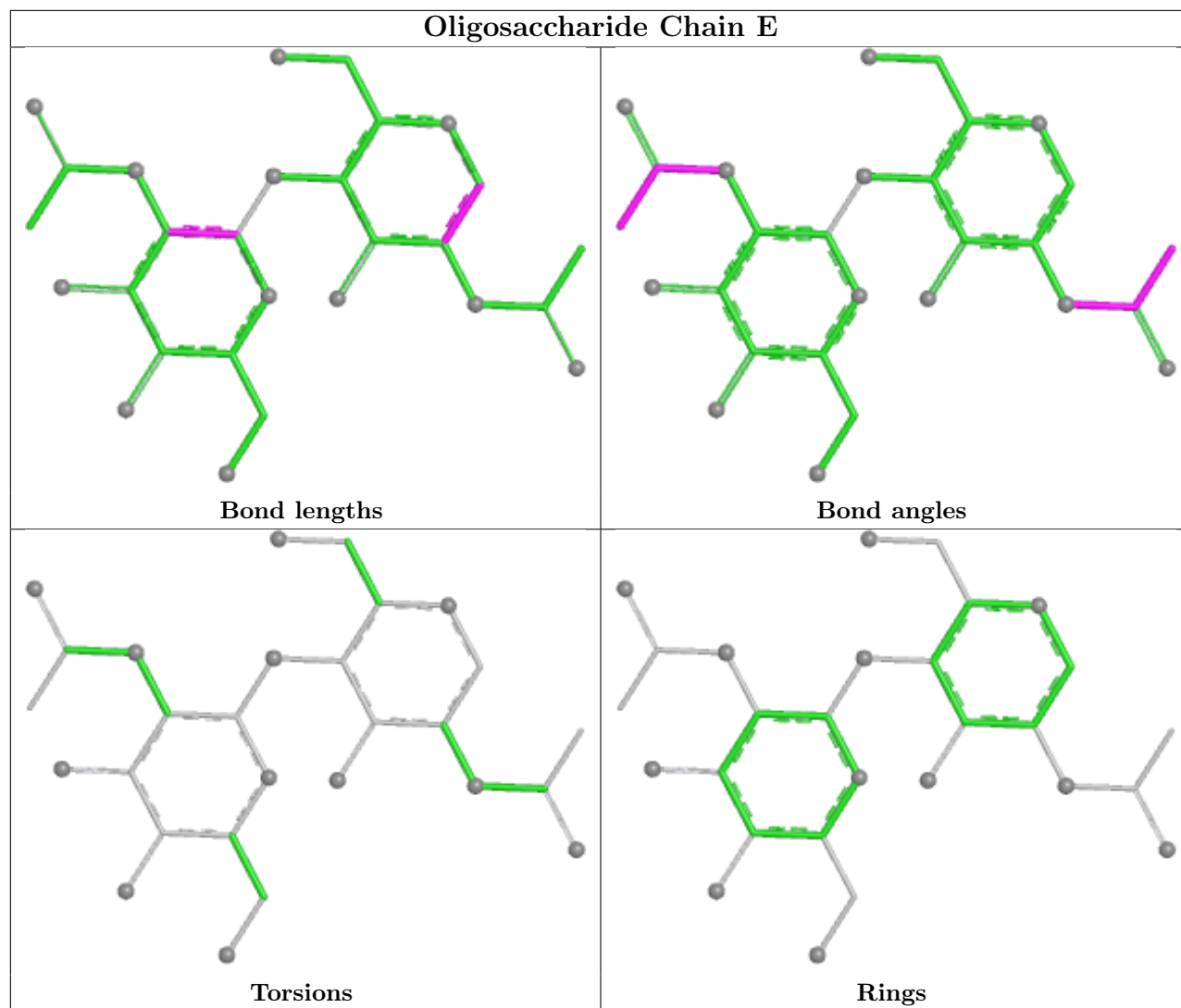
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6

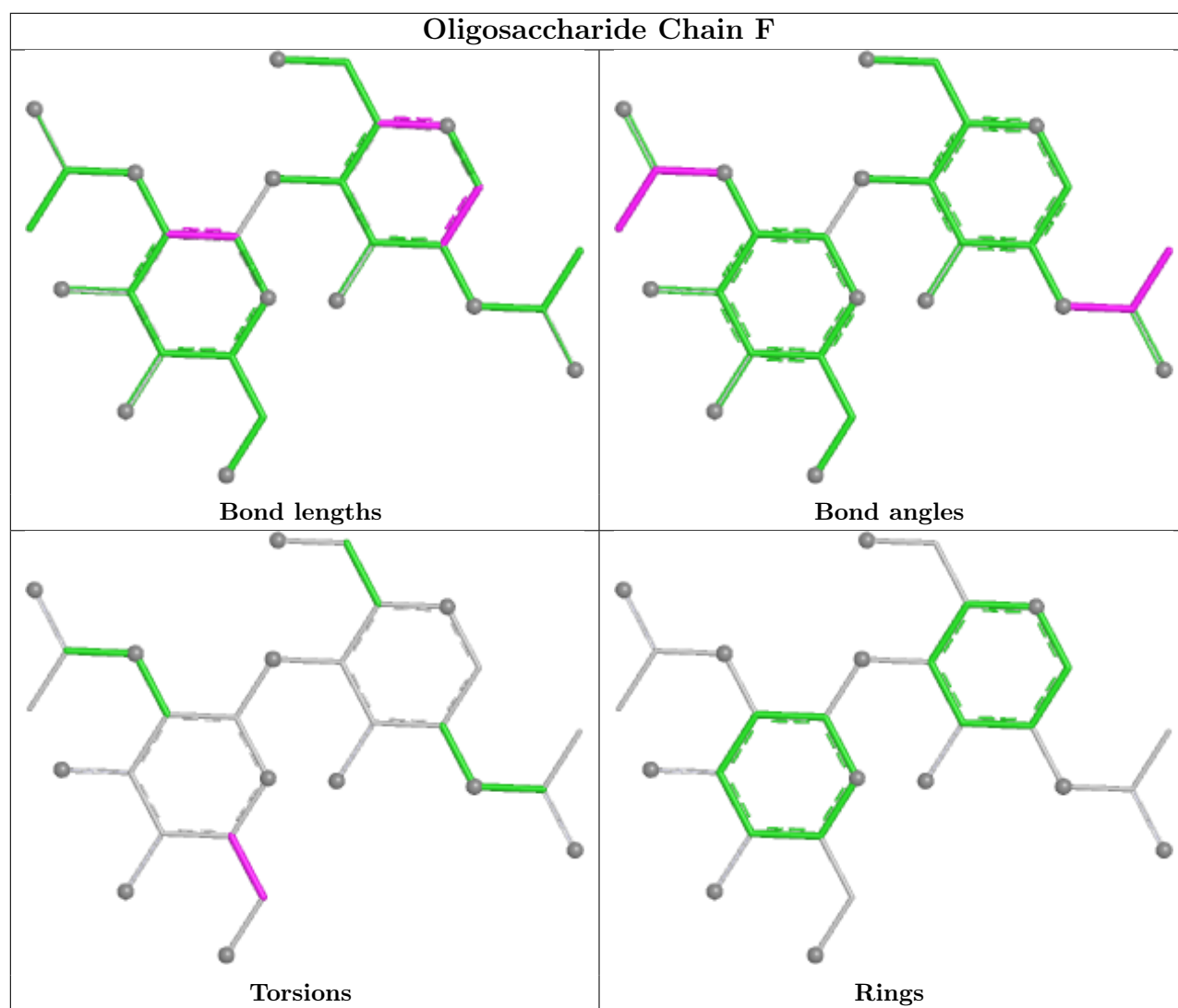
There are no ring outliers.

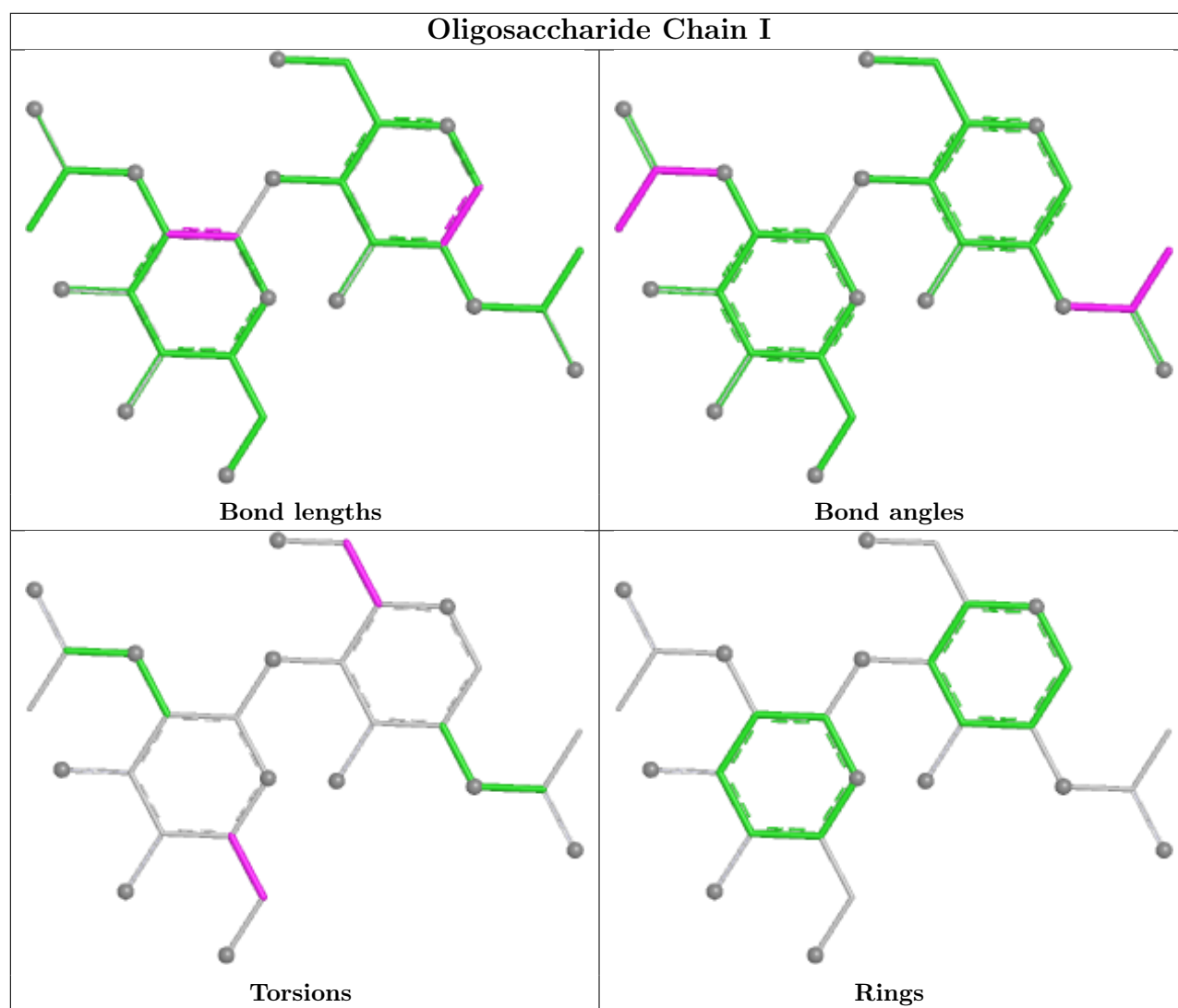
No monomer is involved in short contacts.

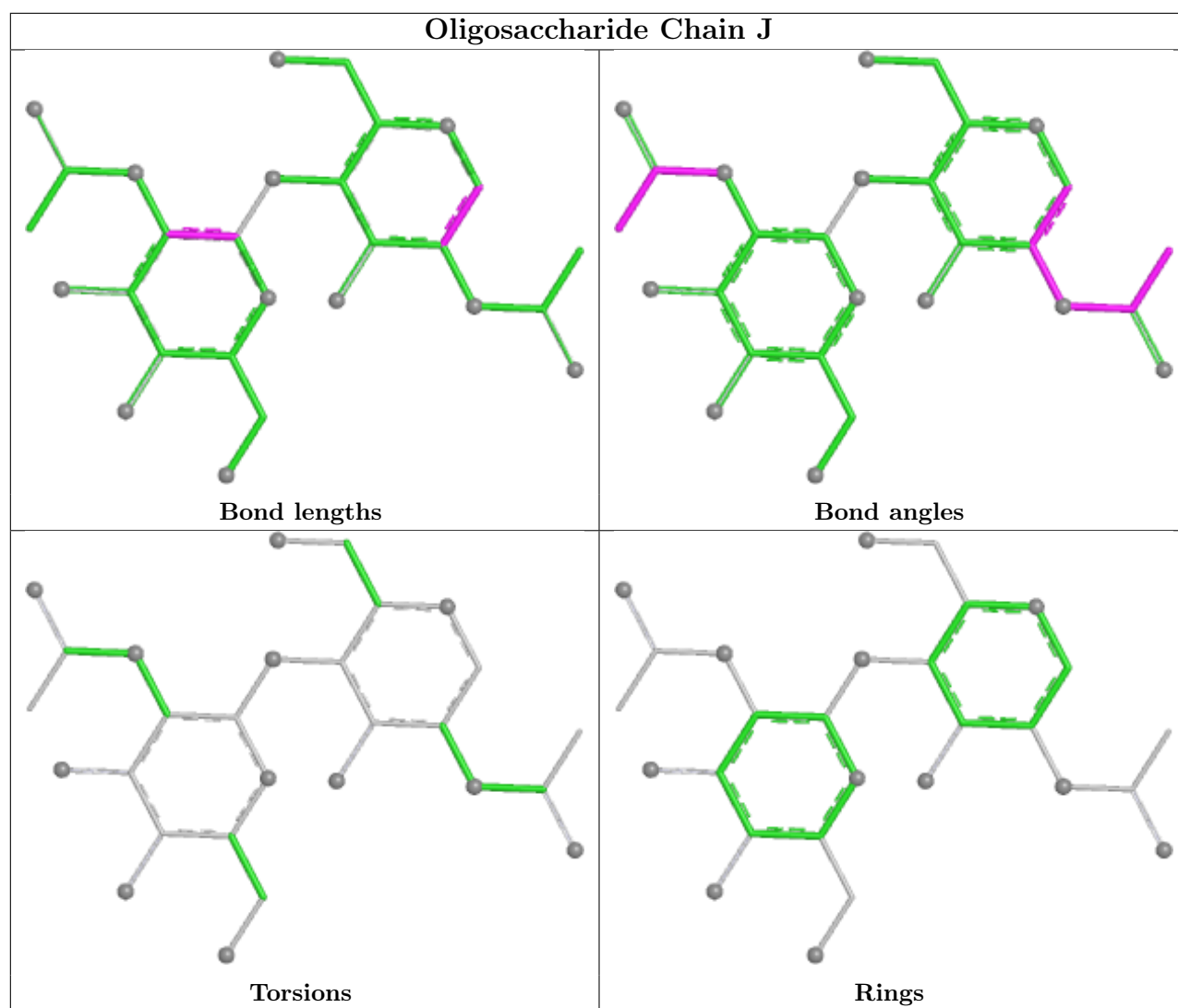
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

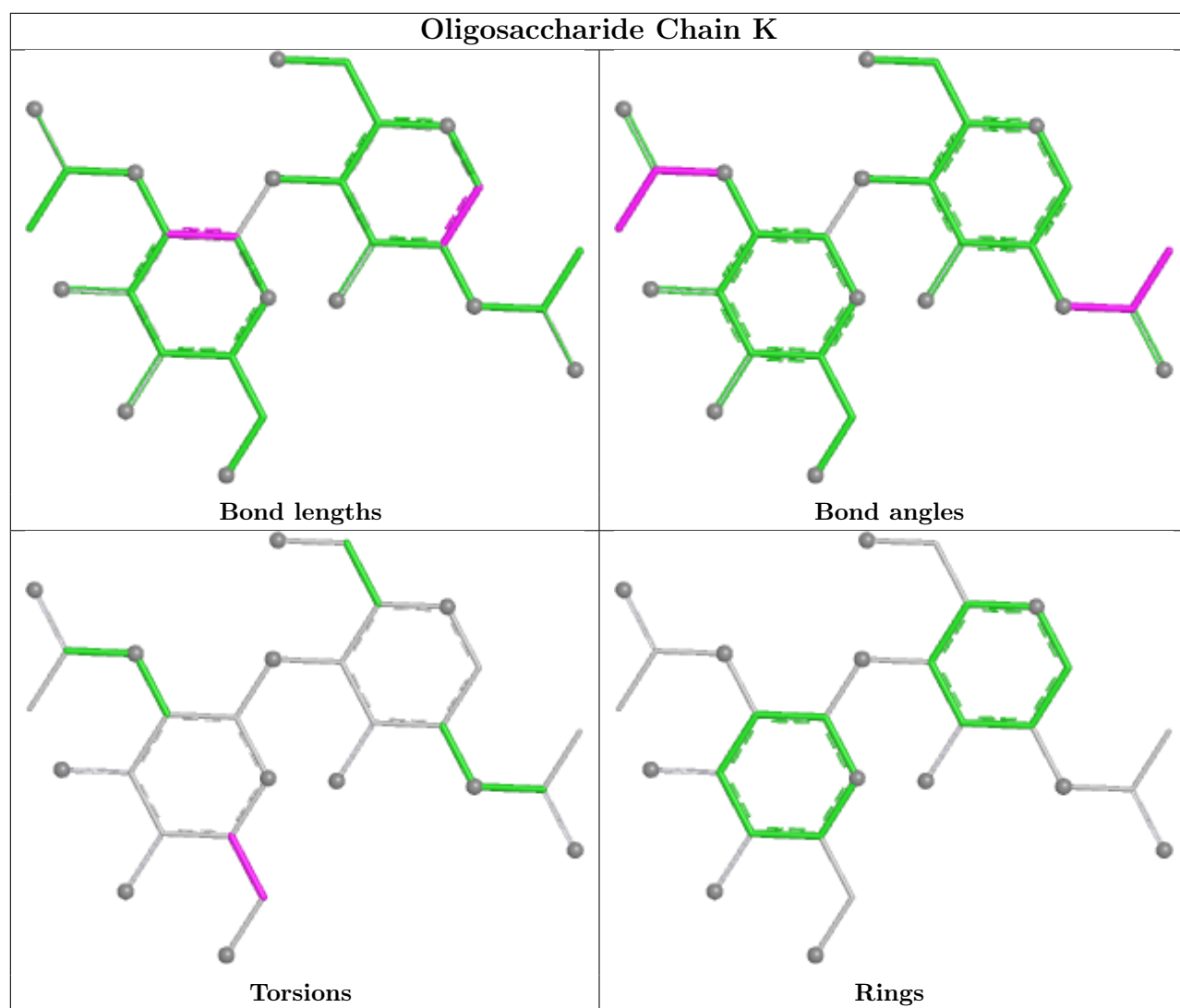


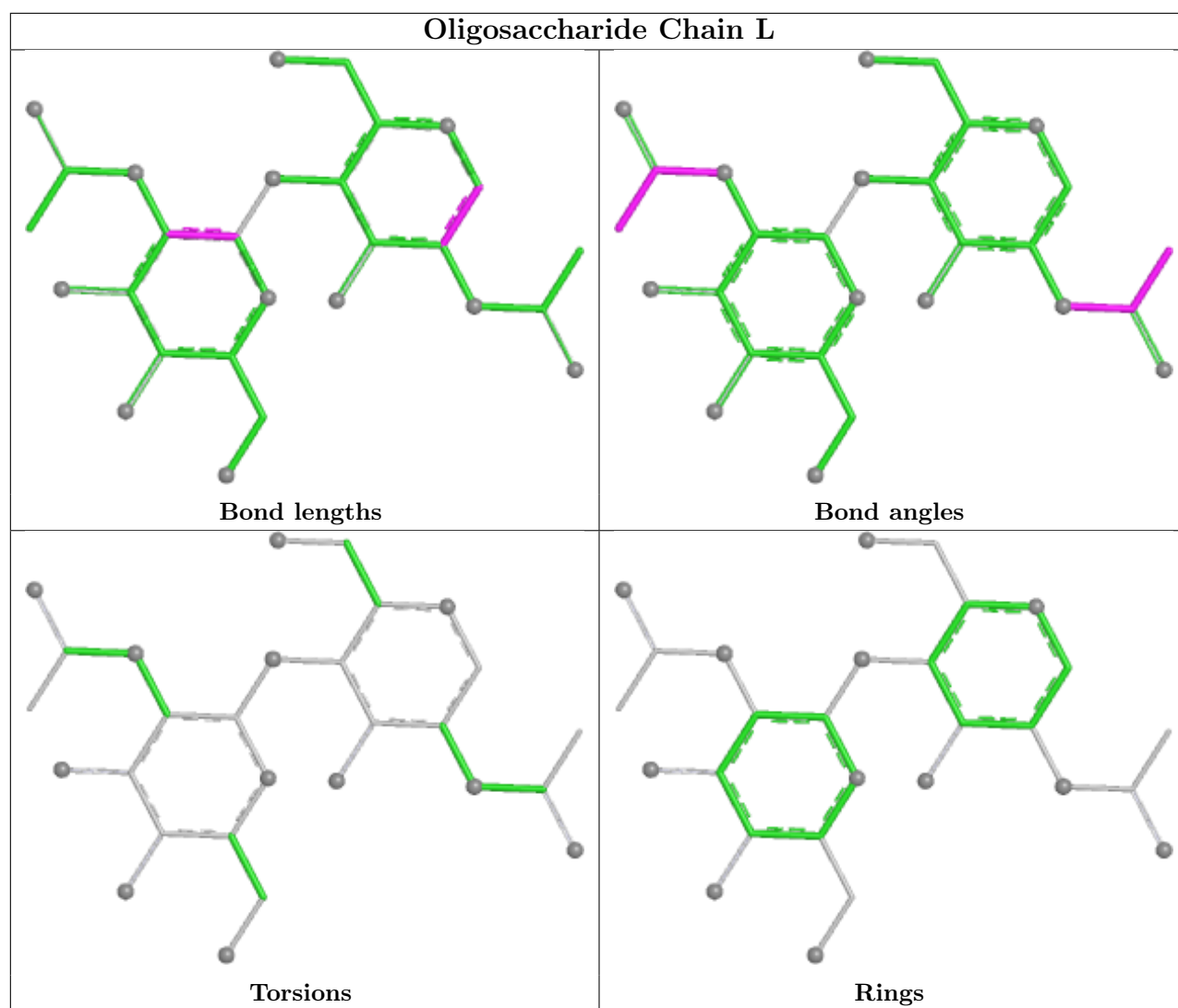


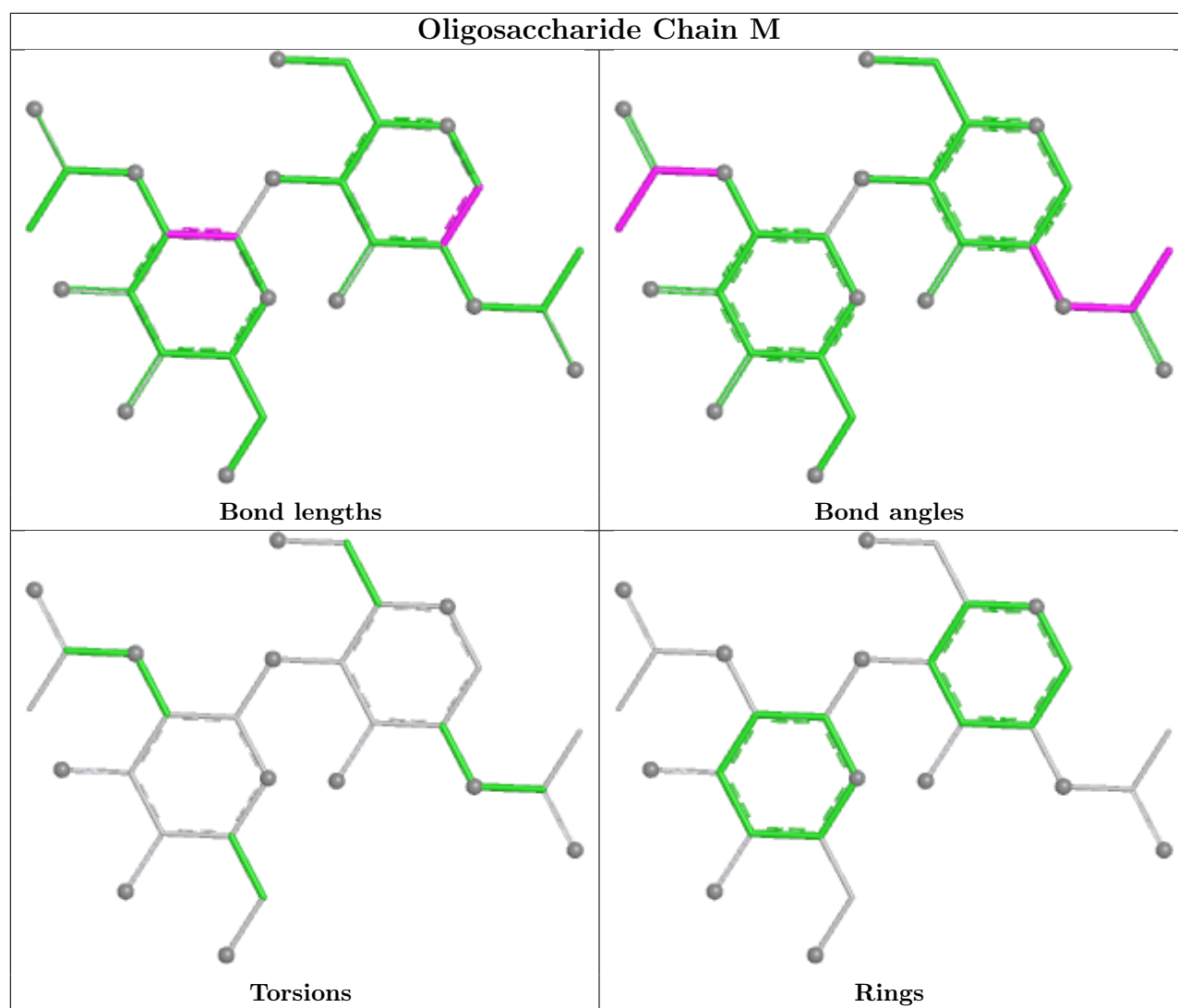


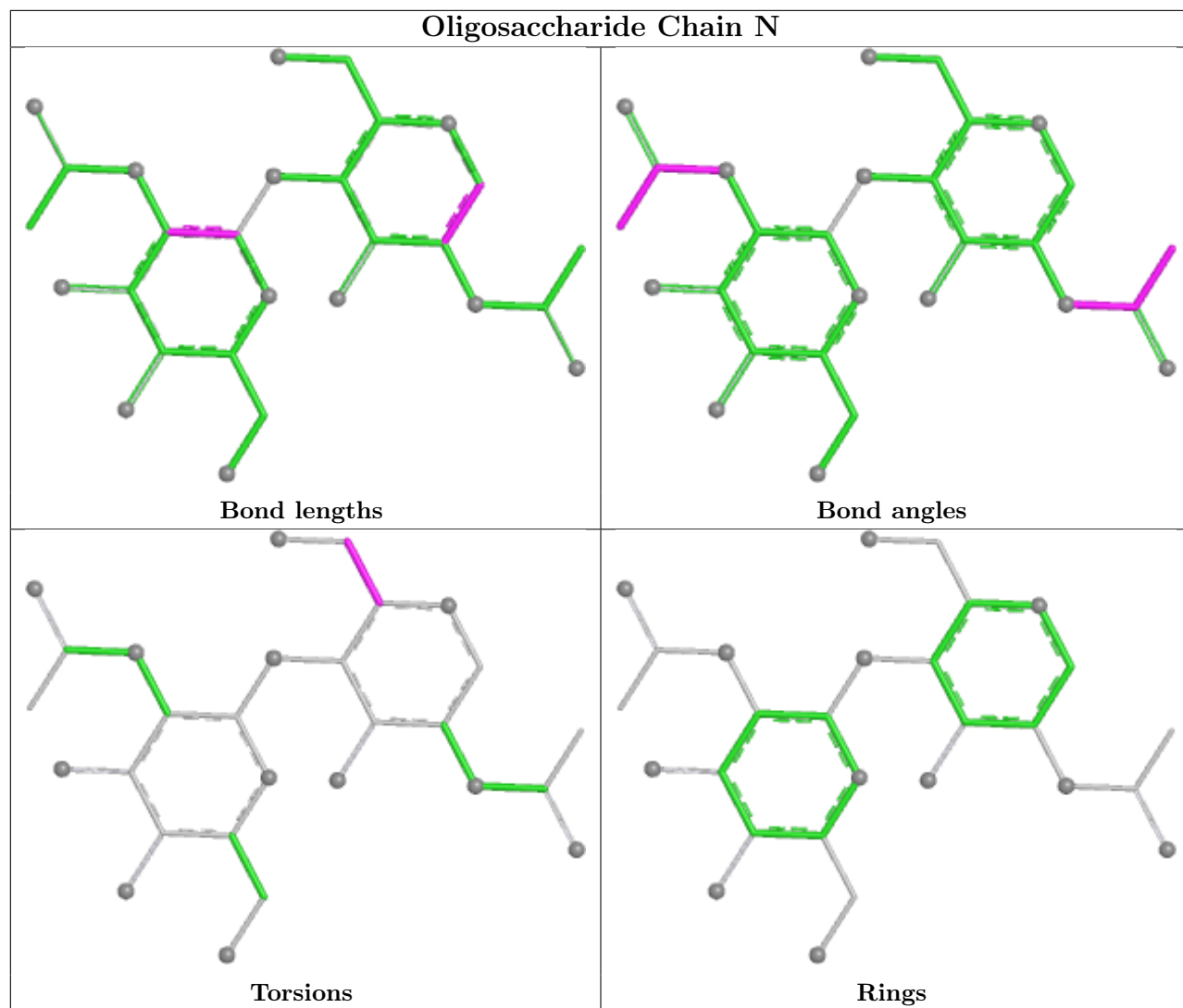


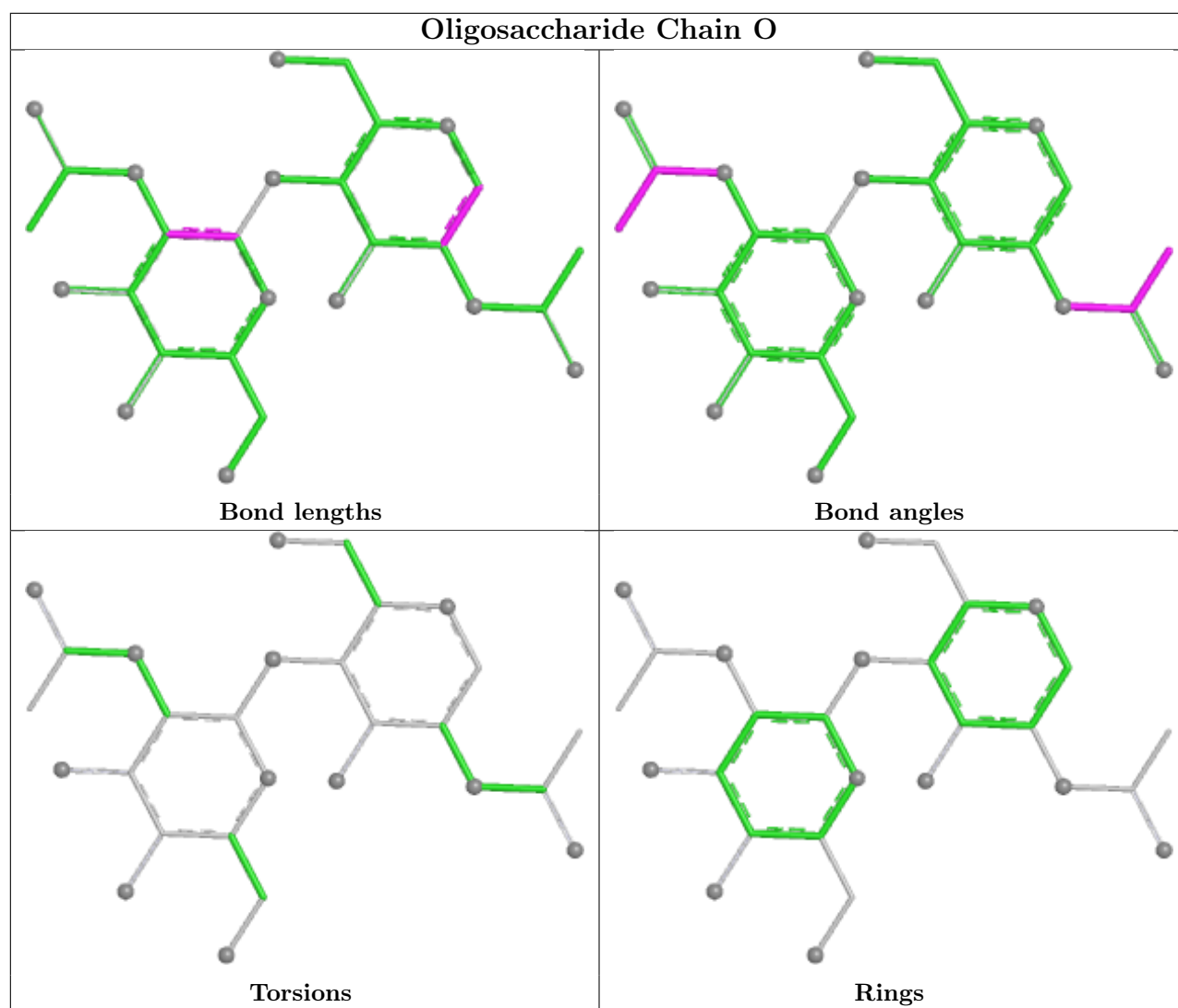


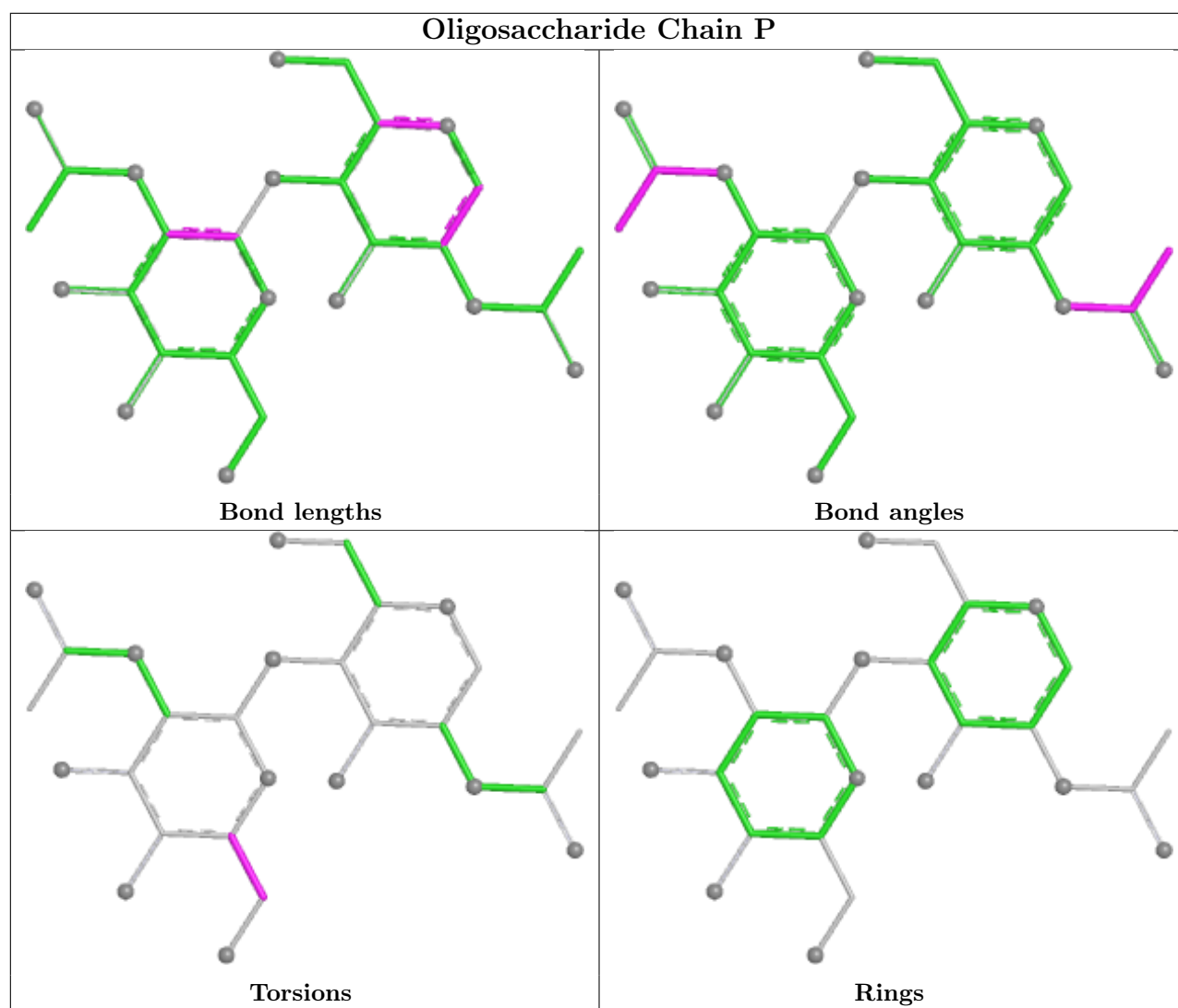


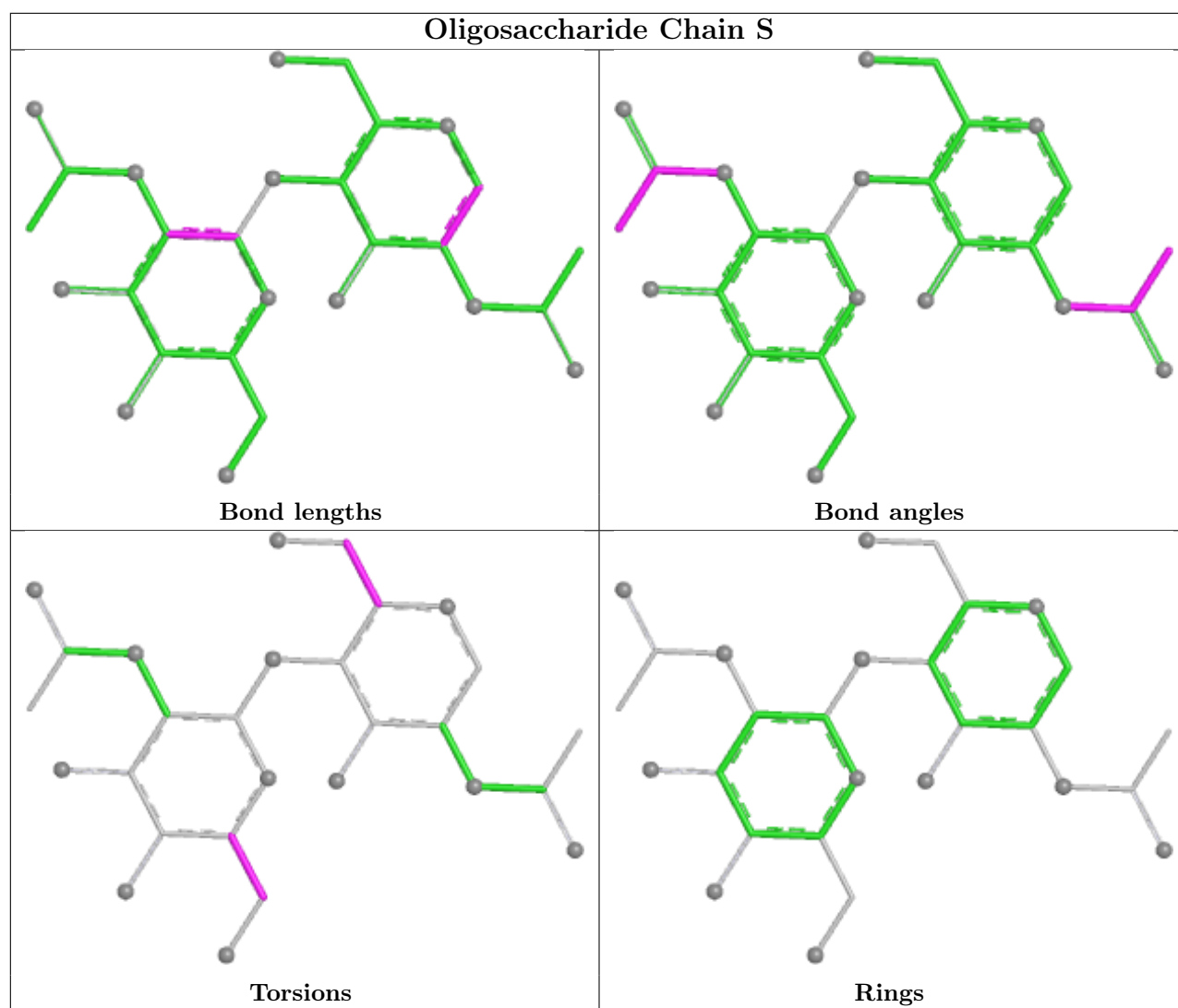


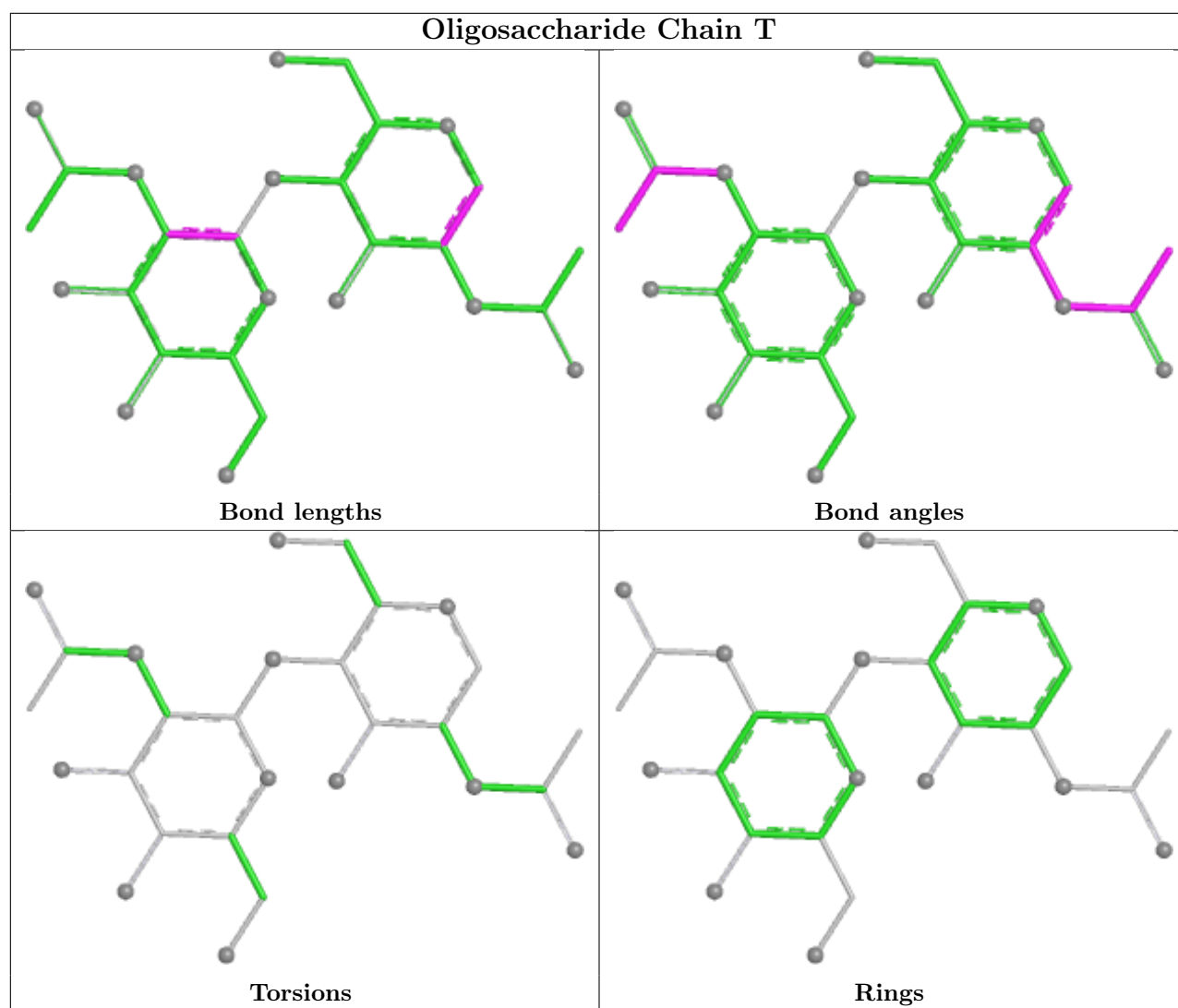


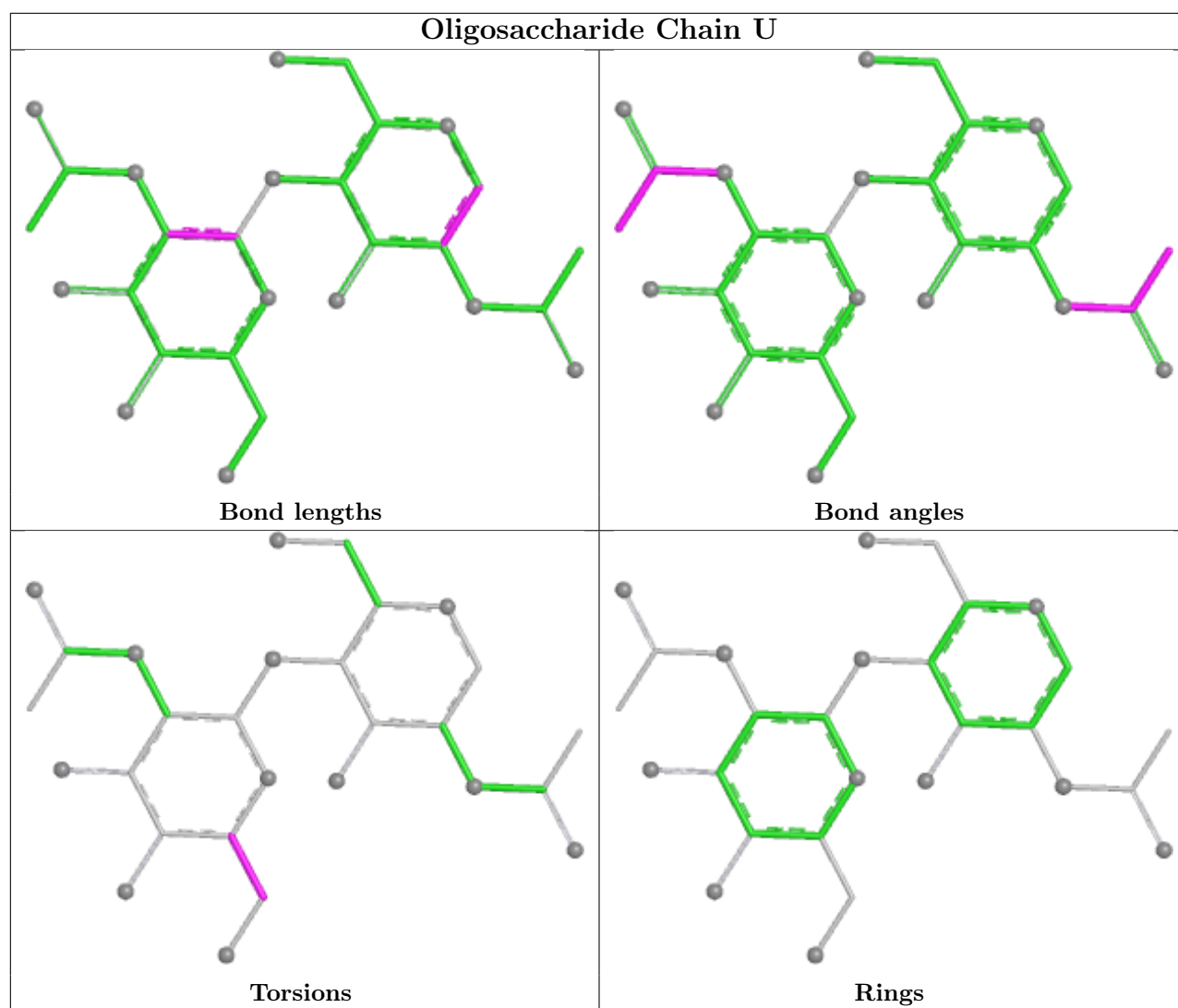


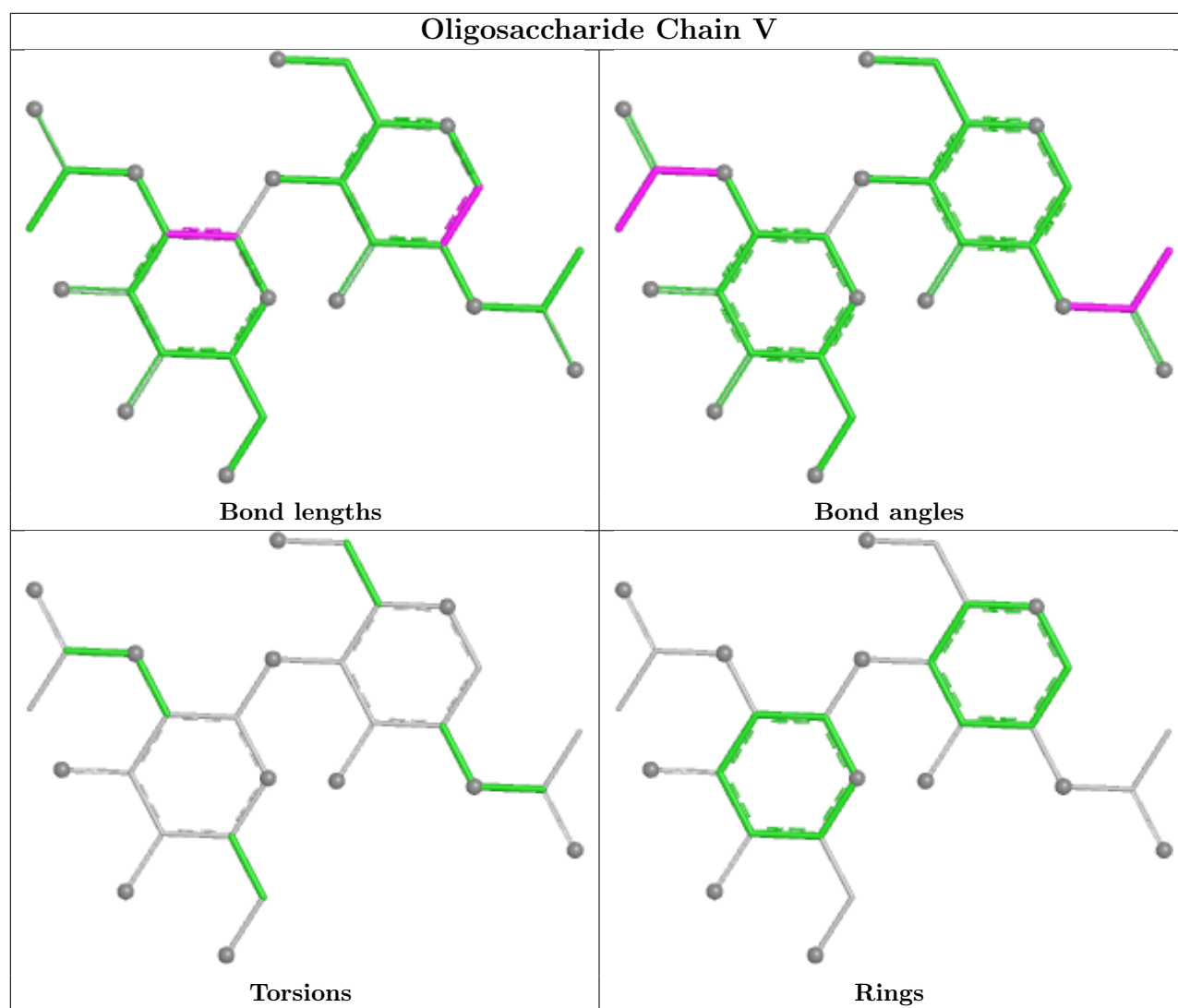


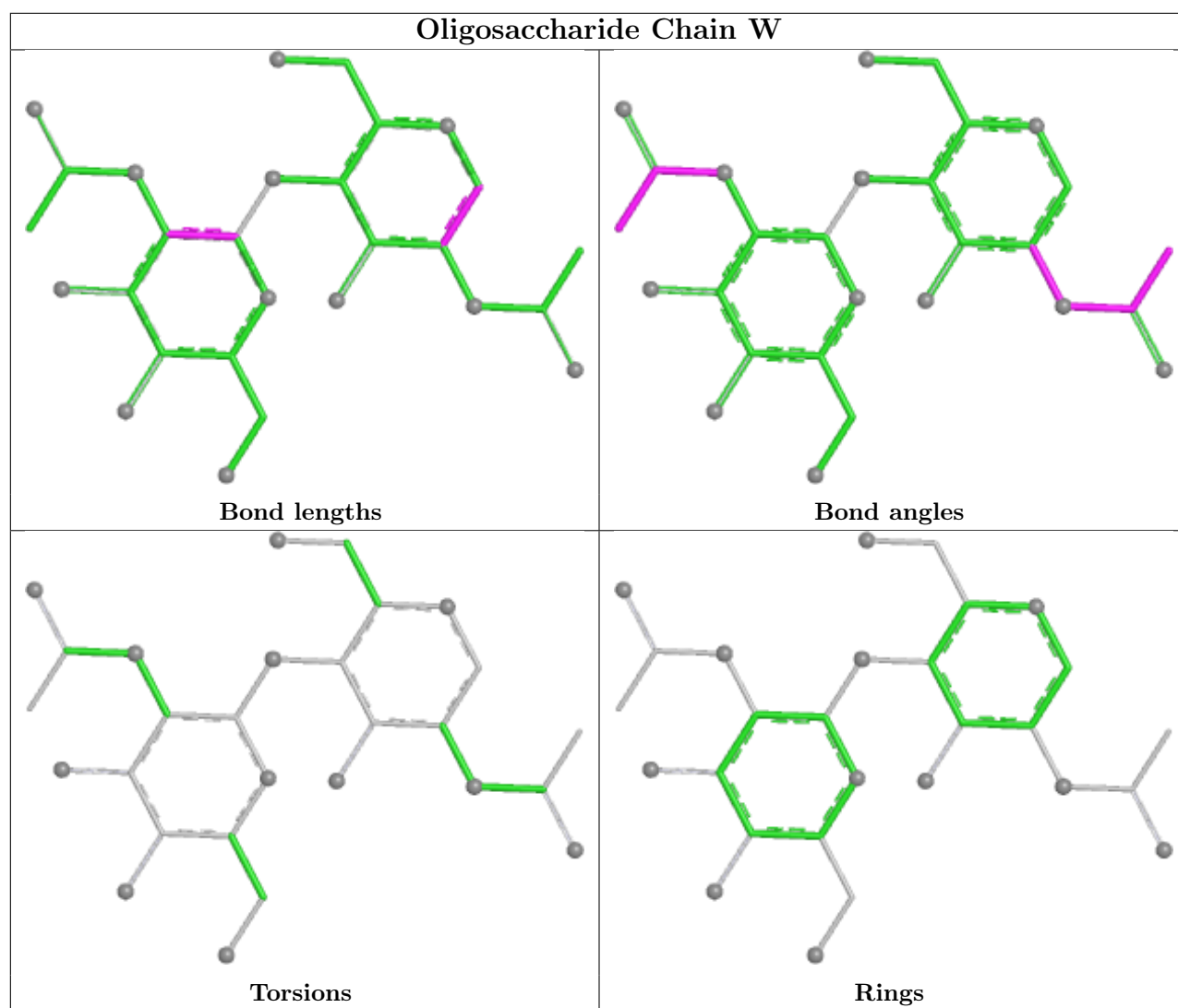


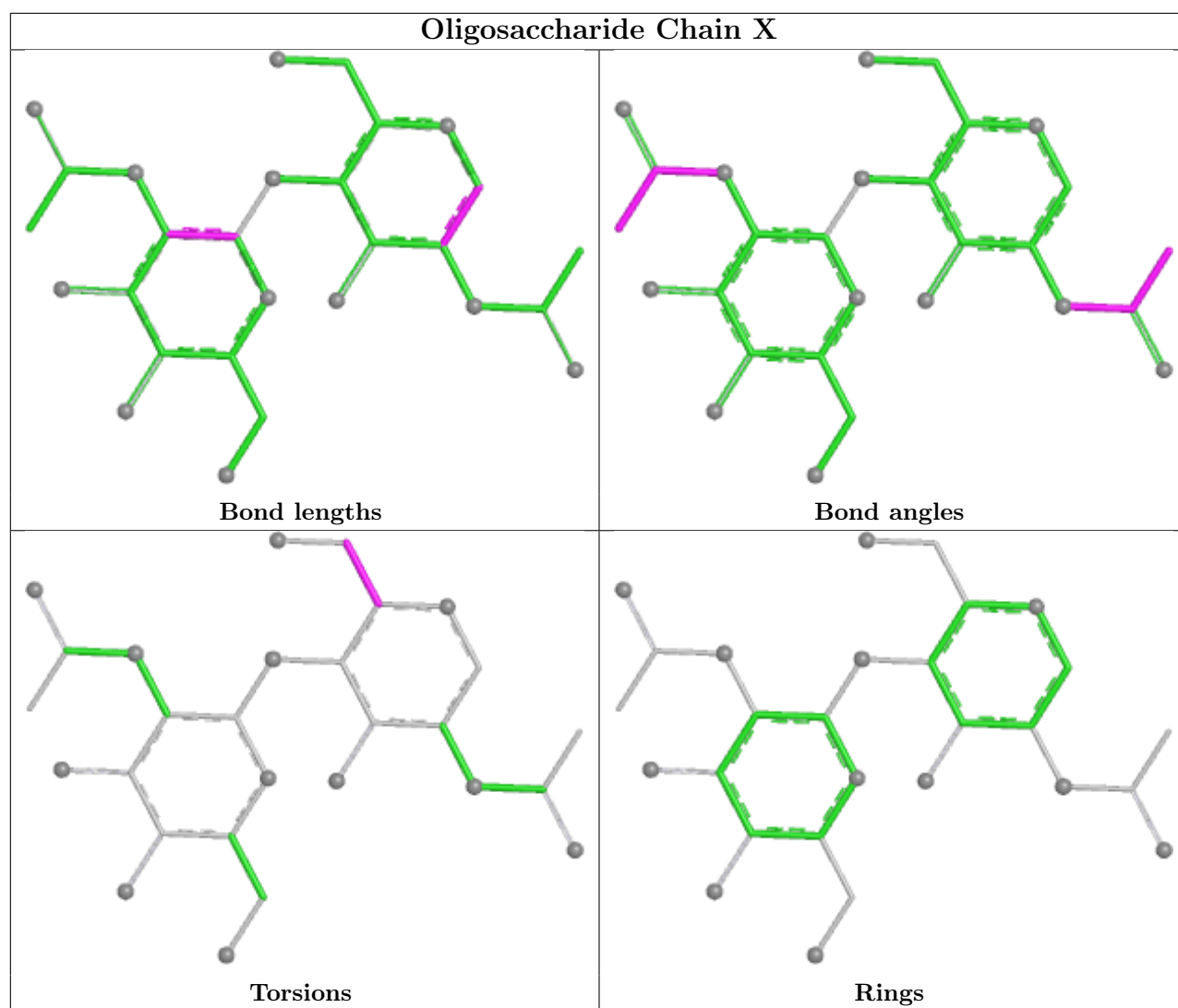


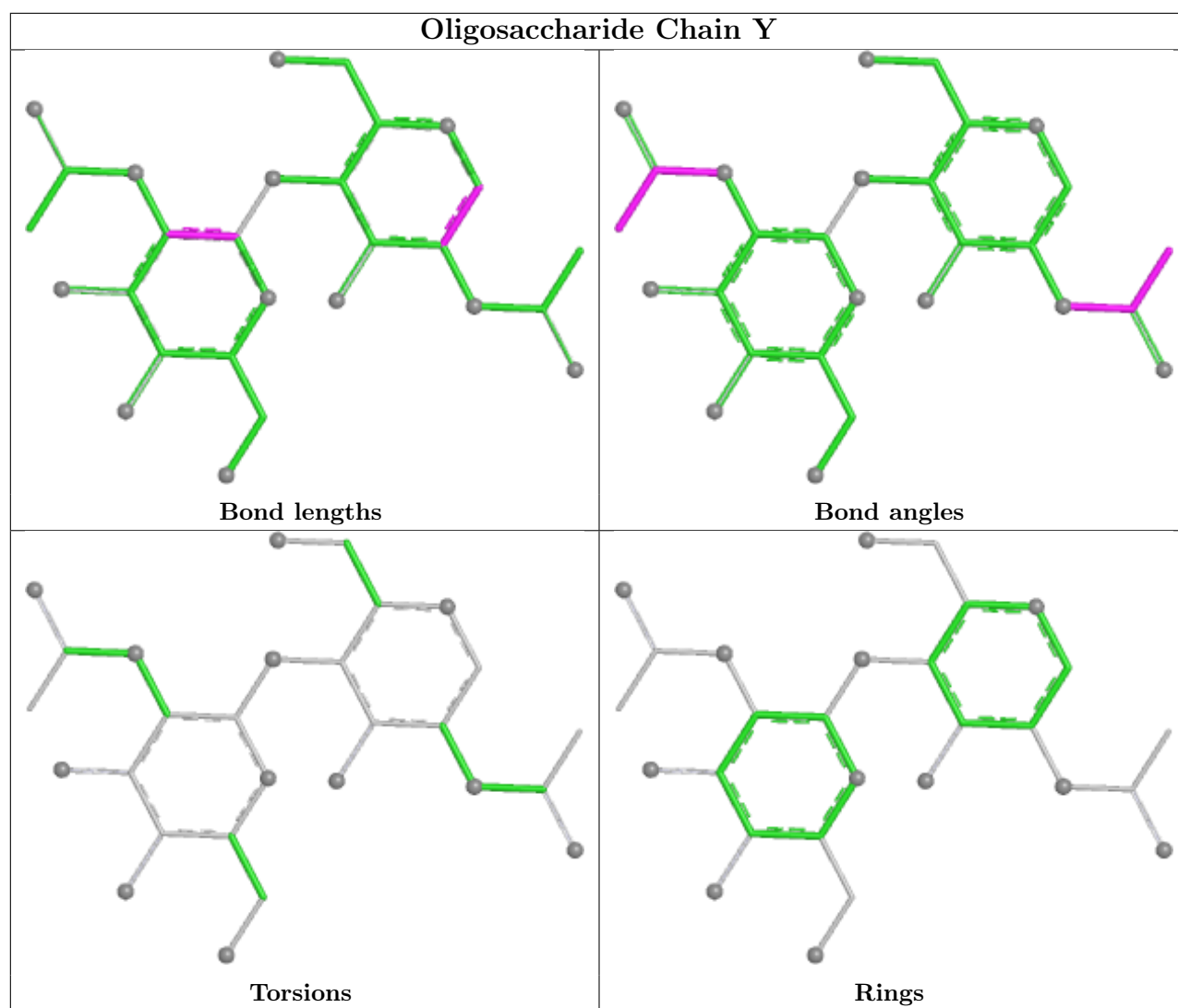


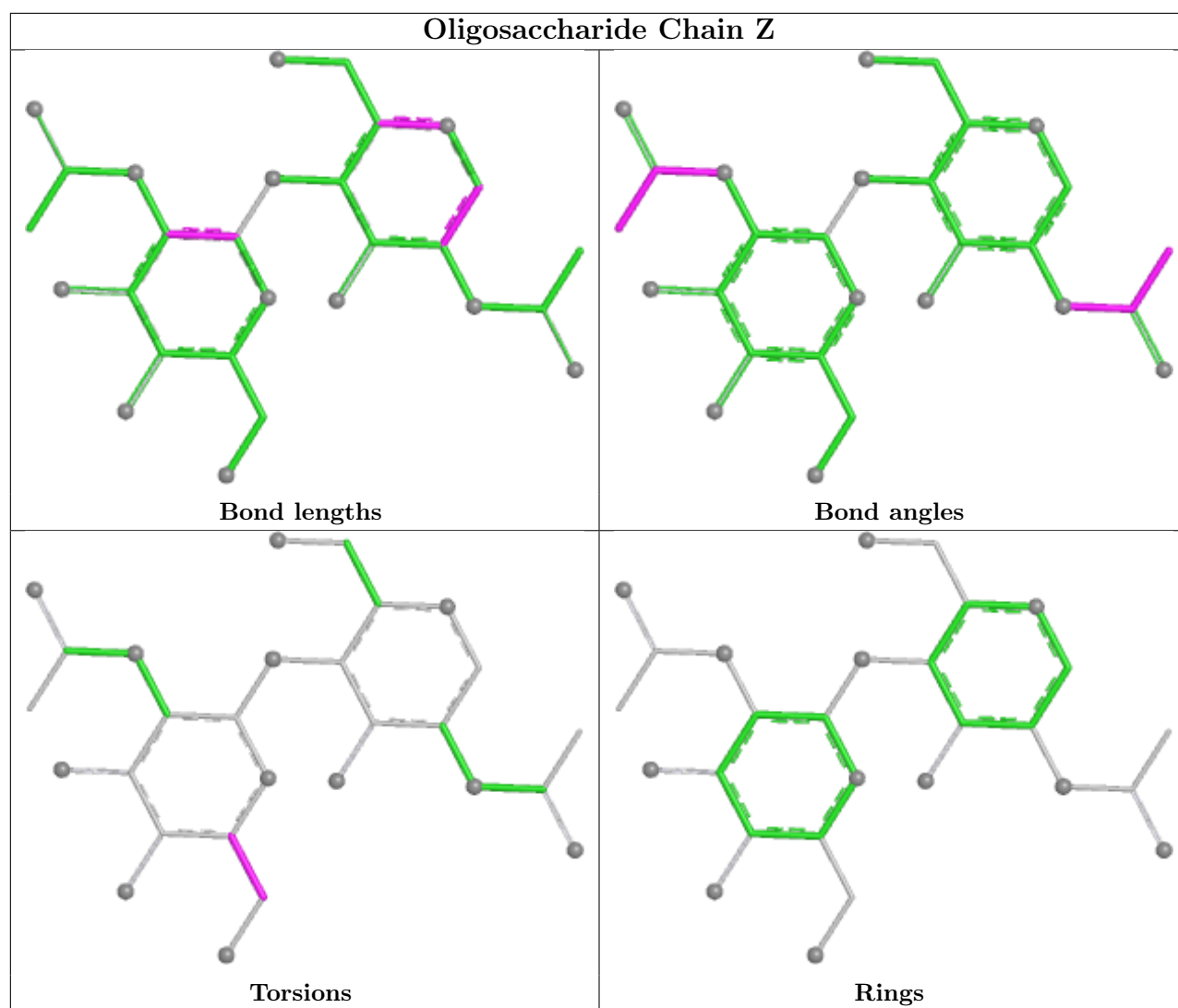


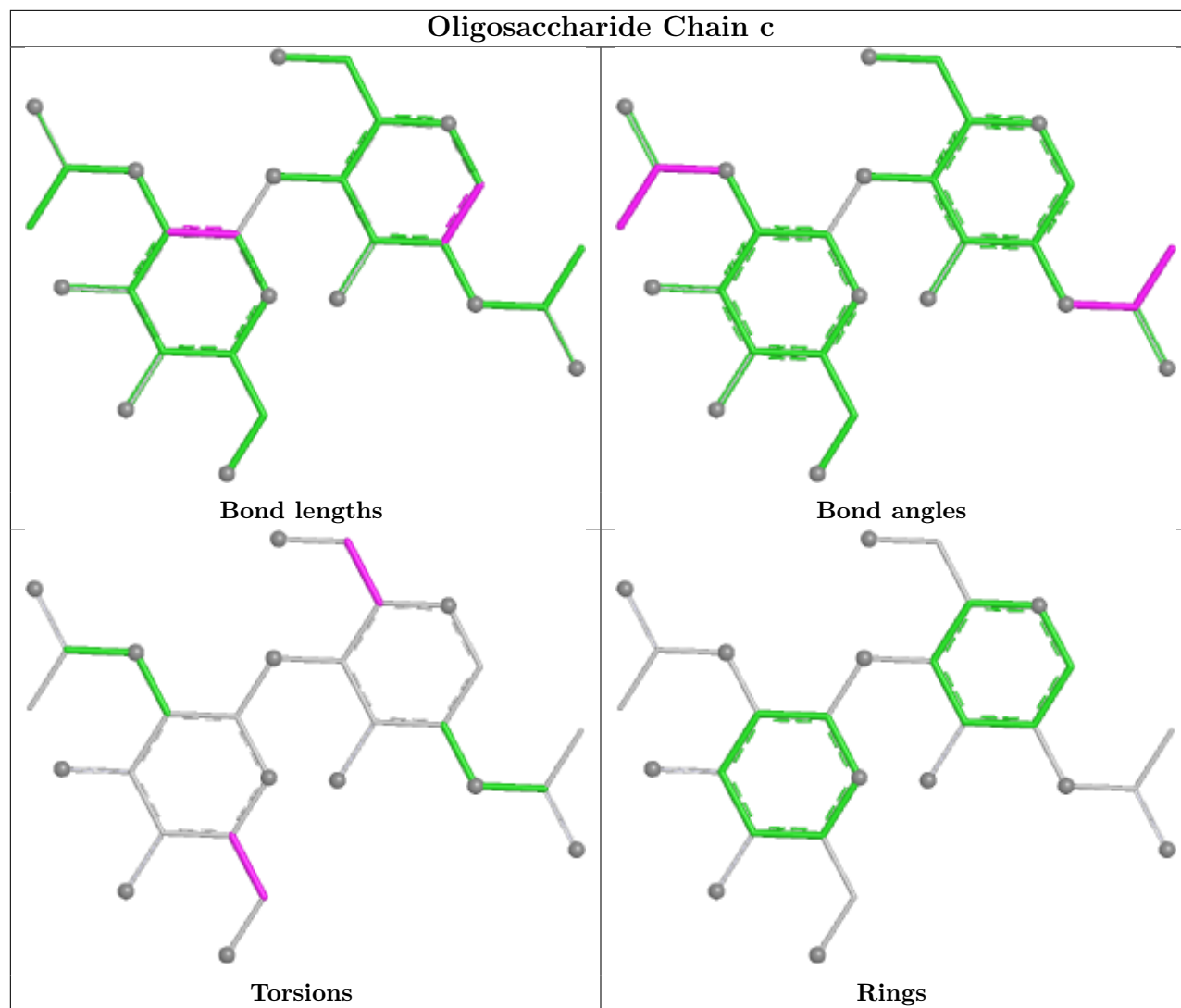


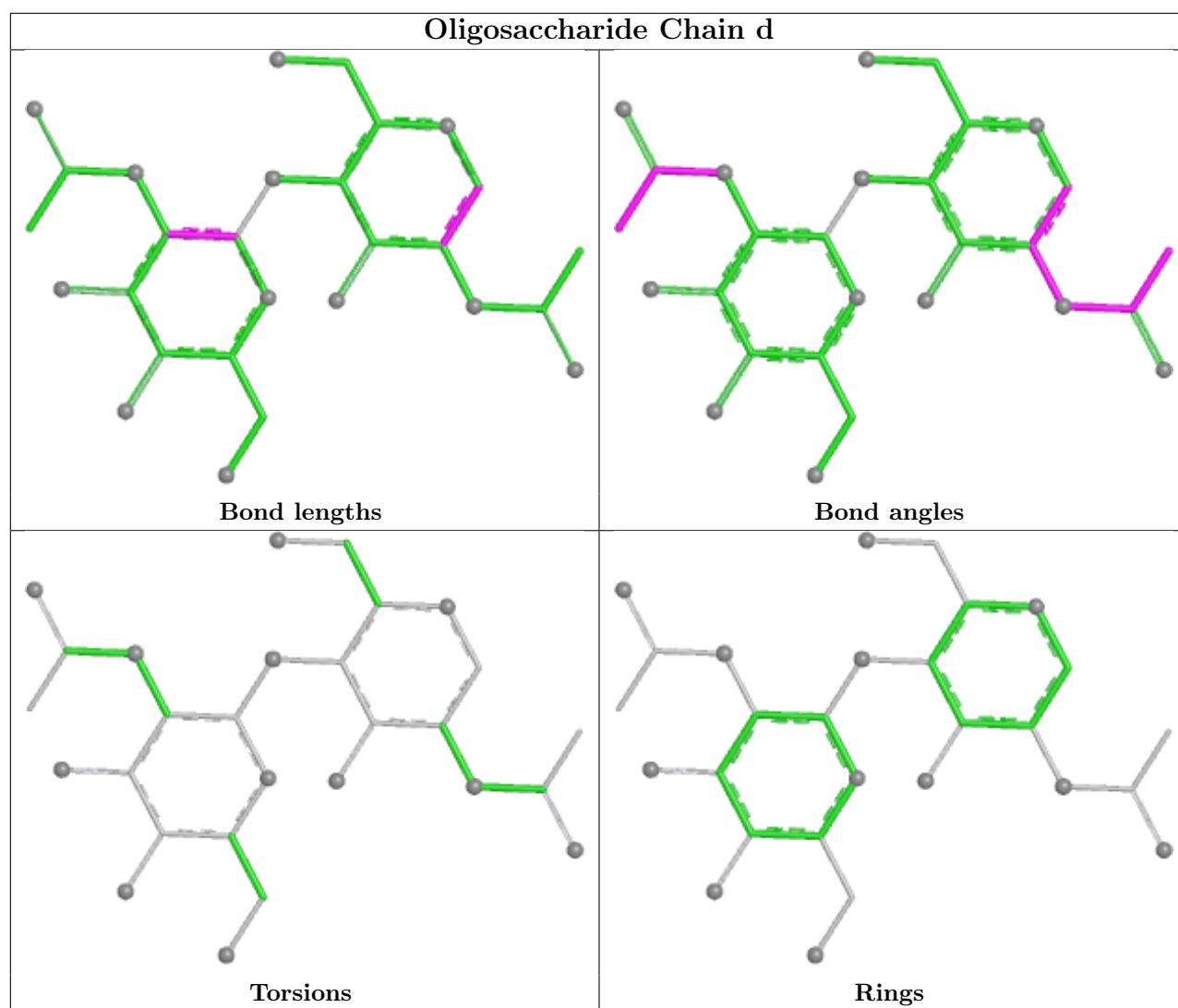


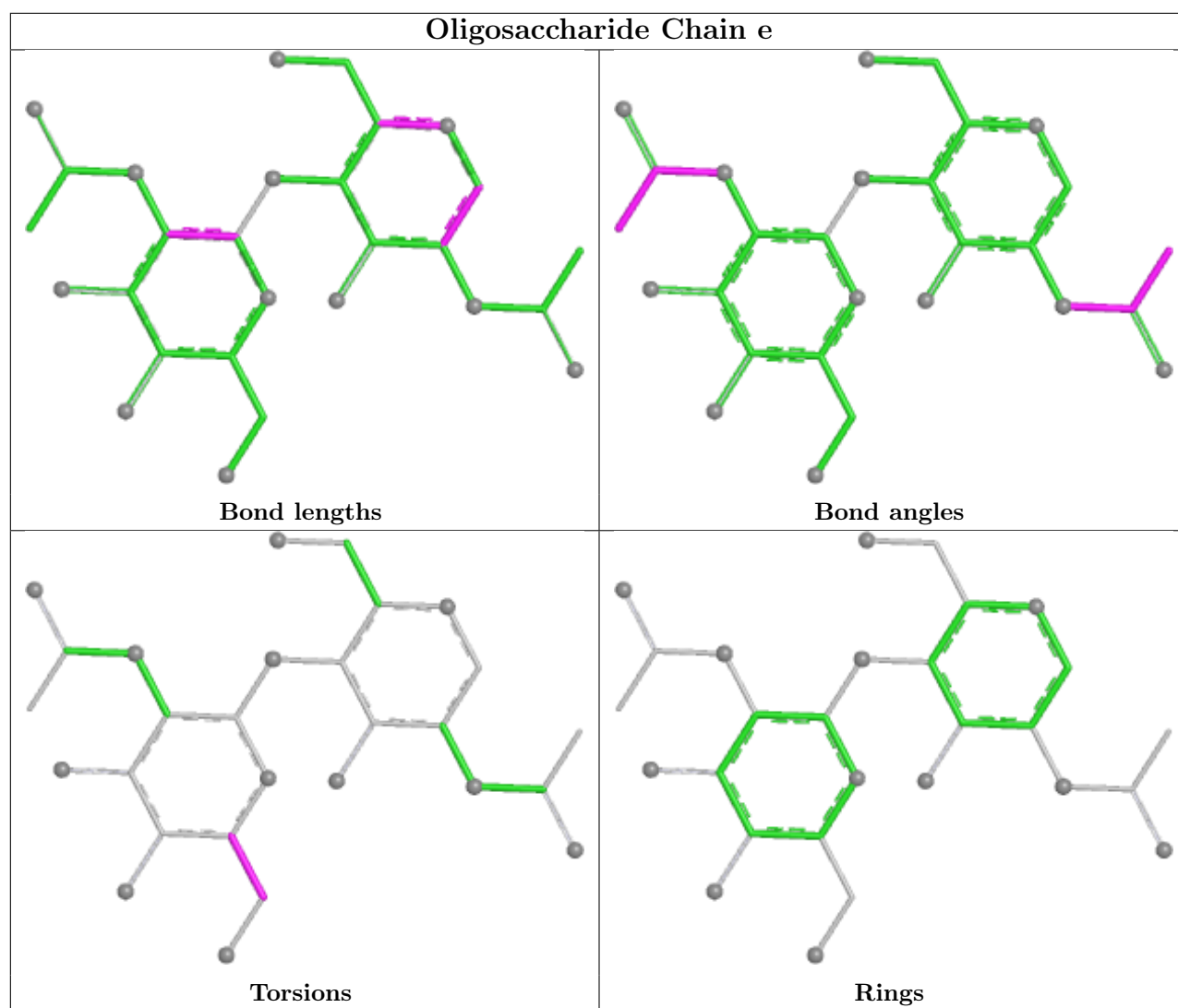


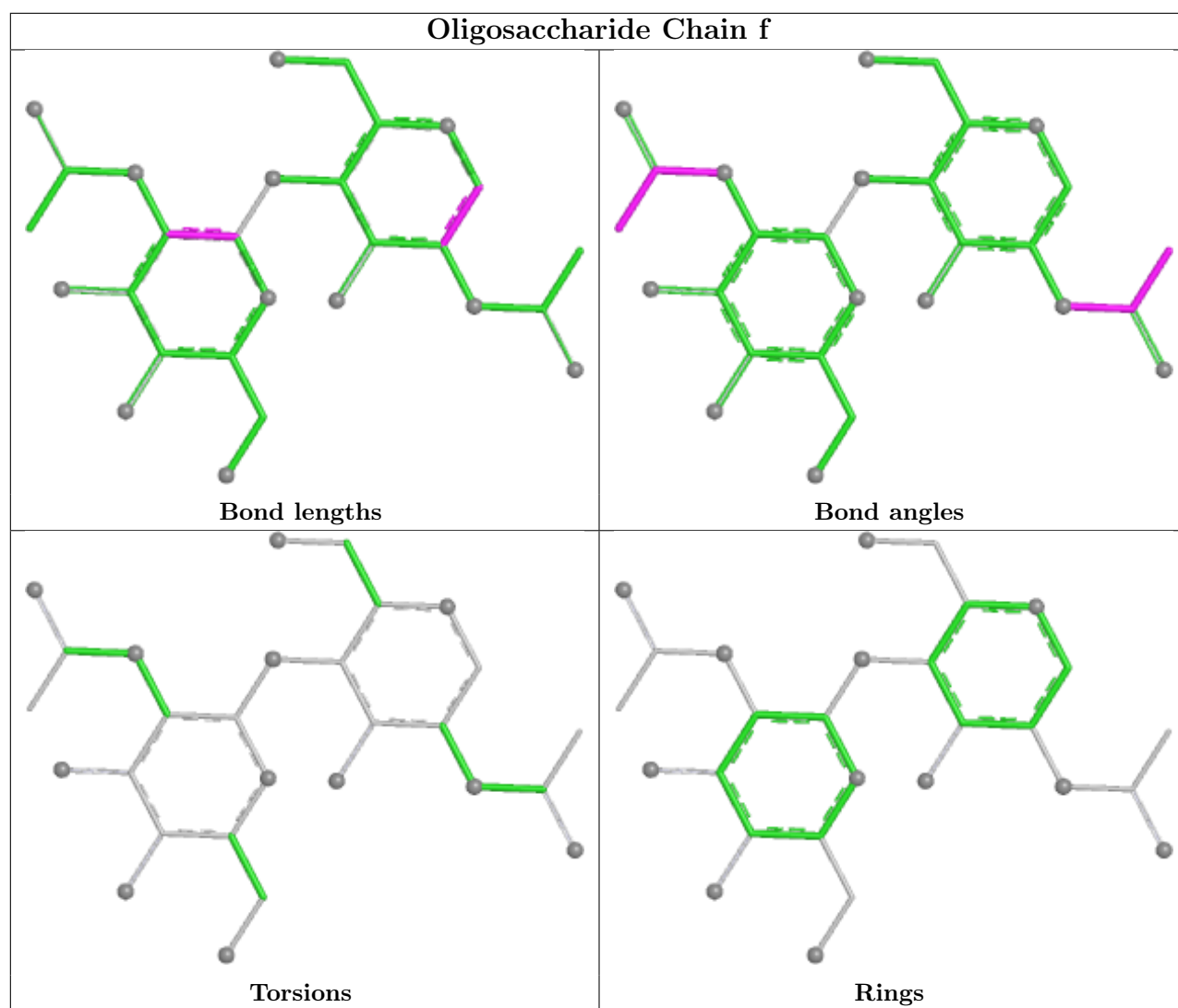


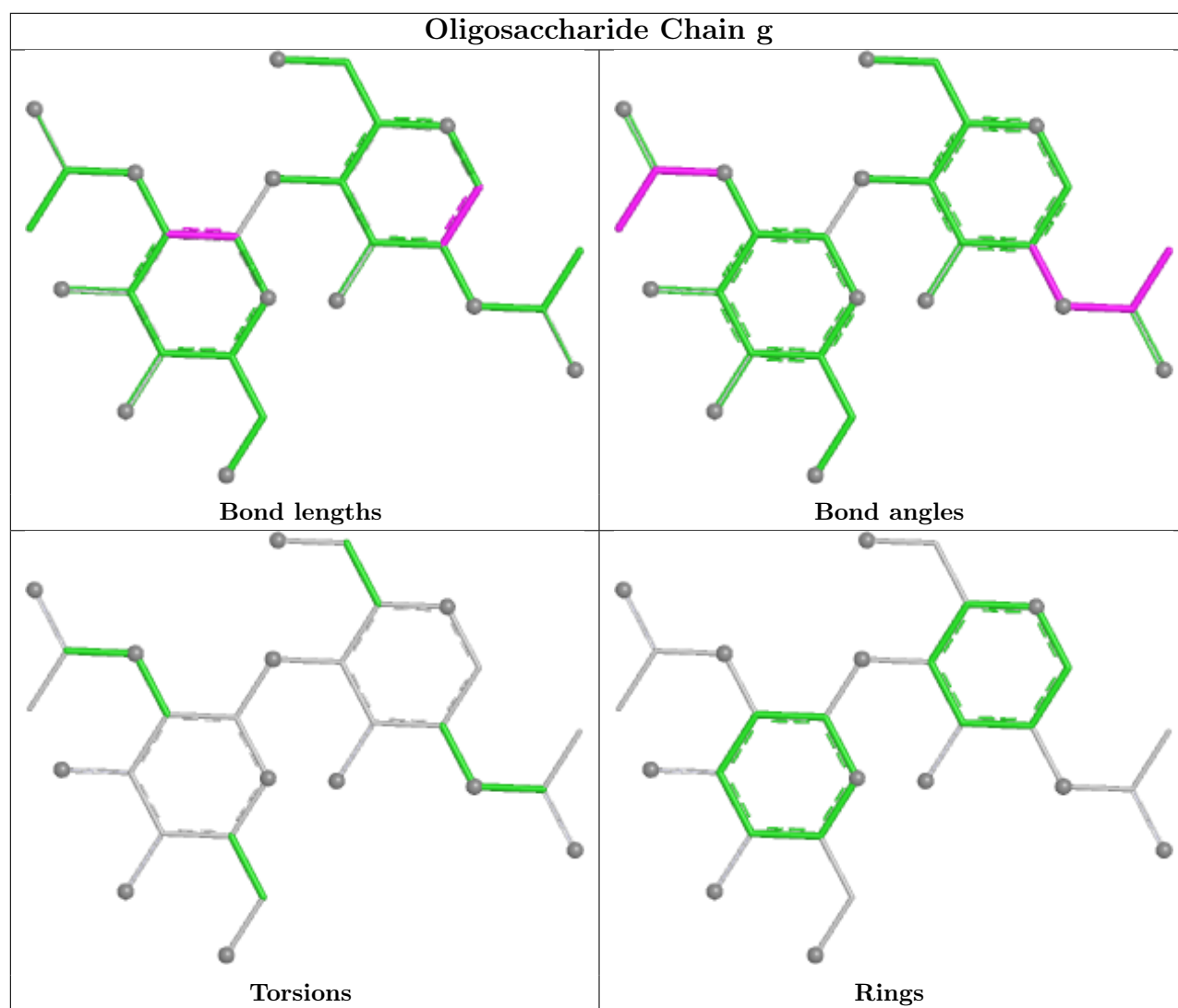


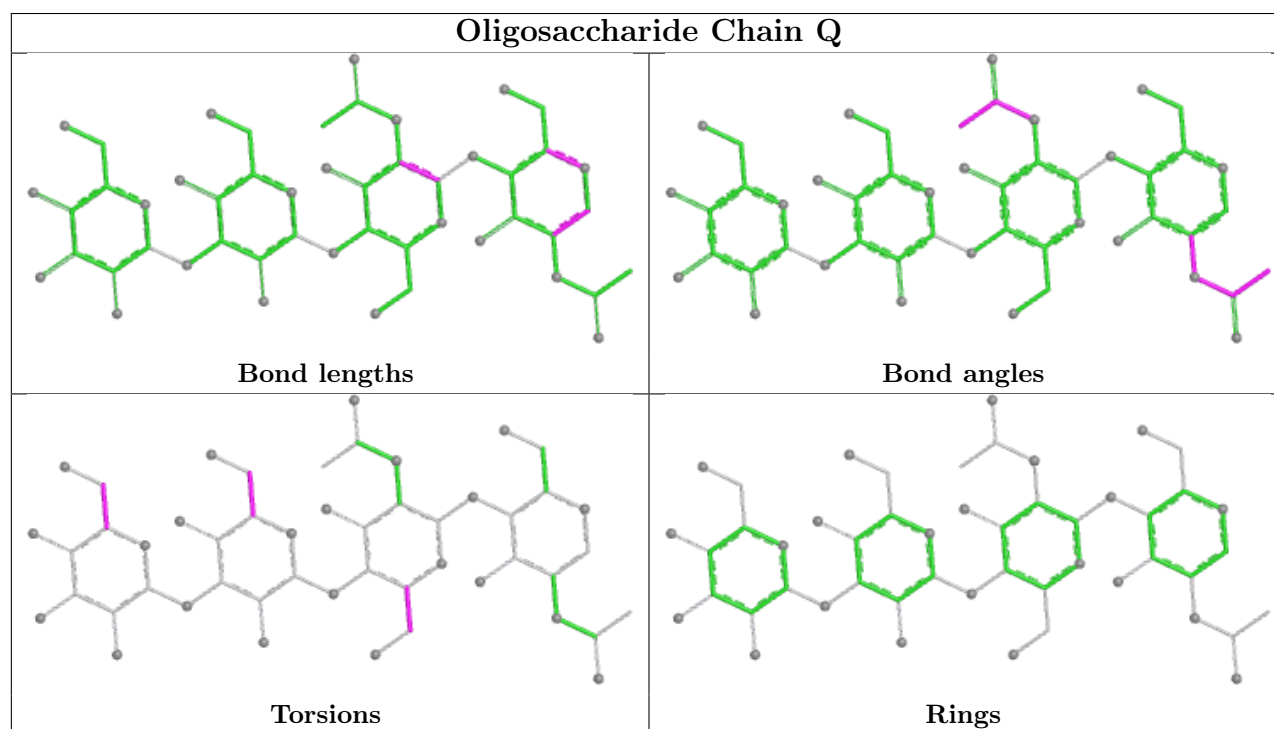
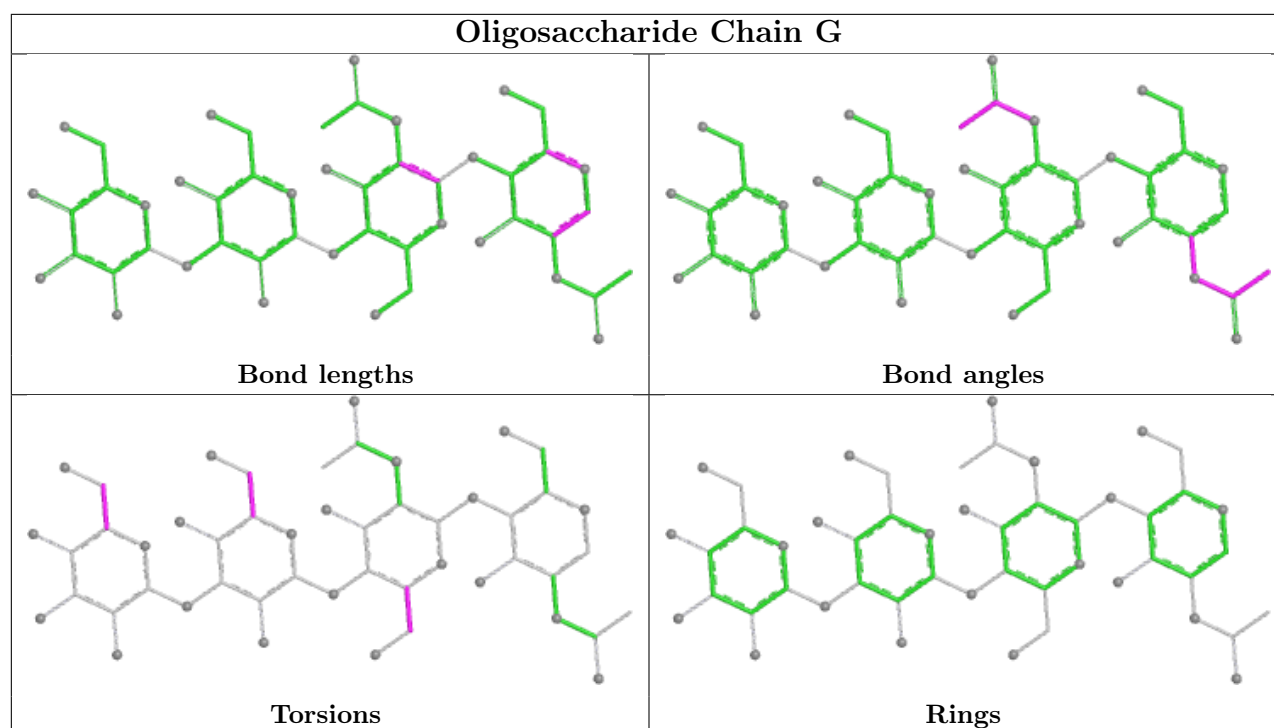


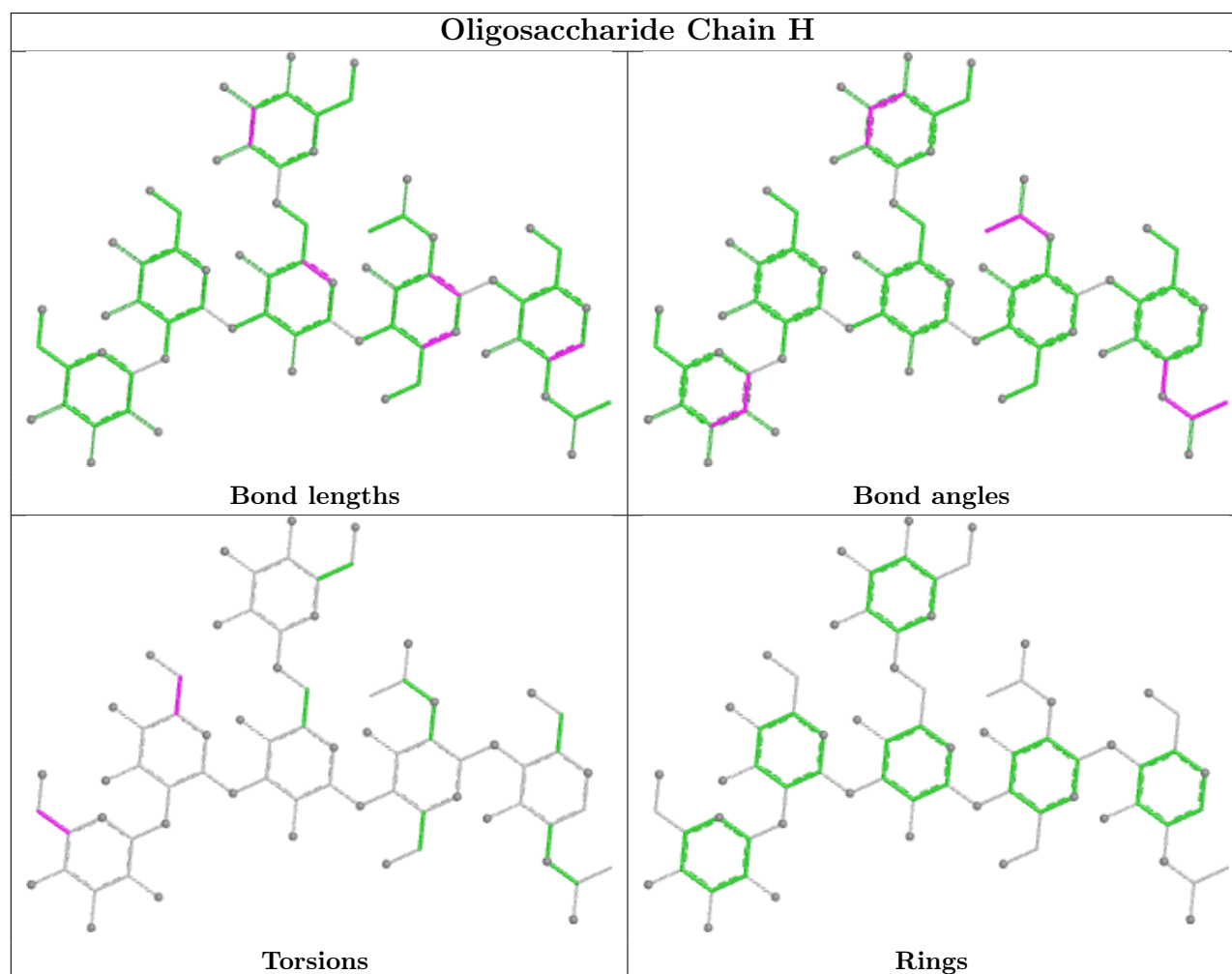
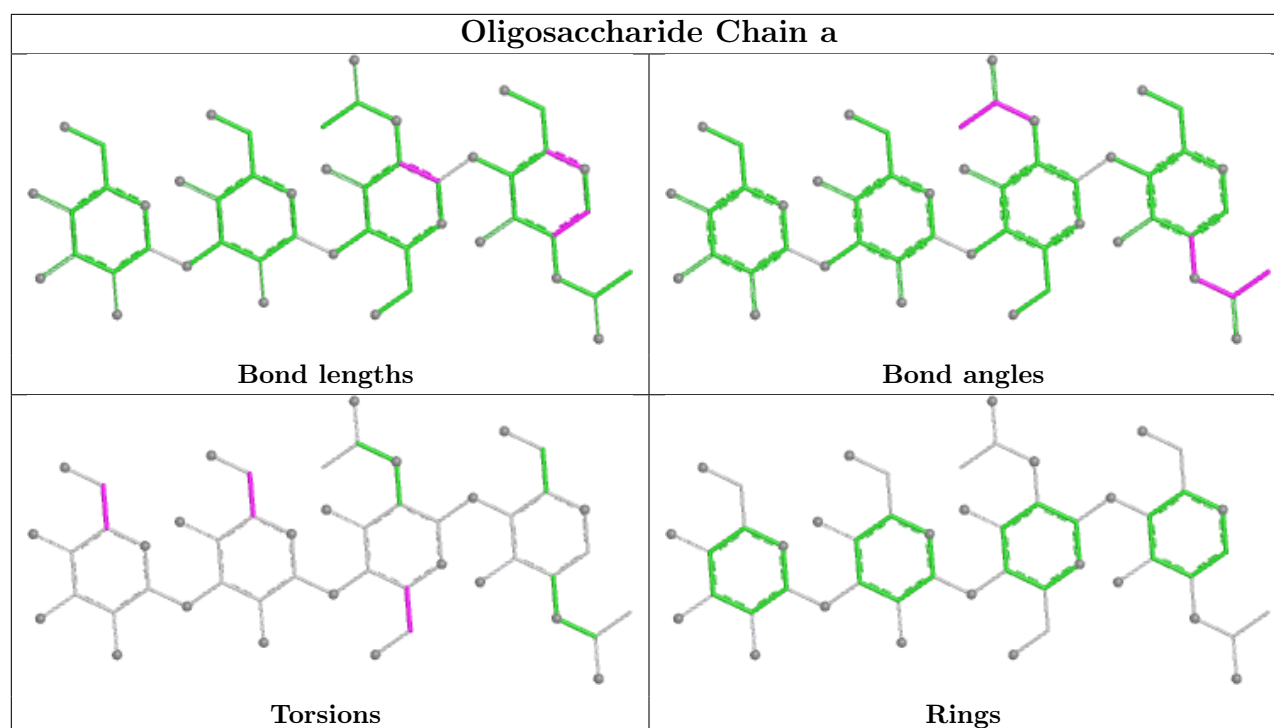


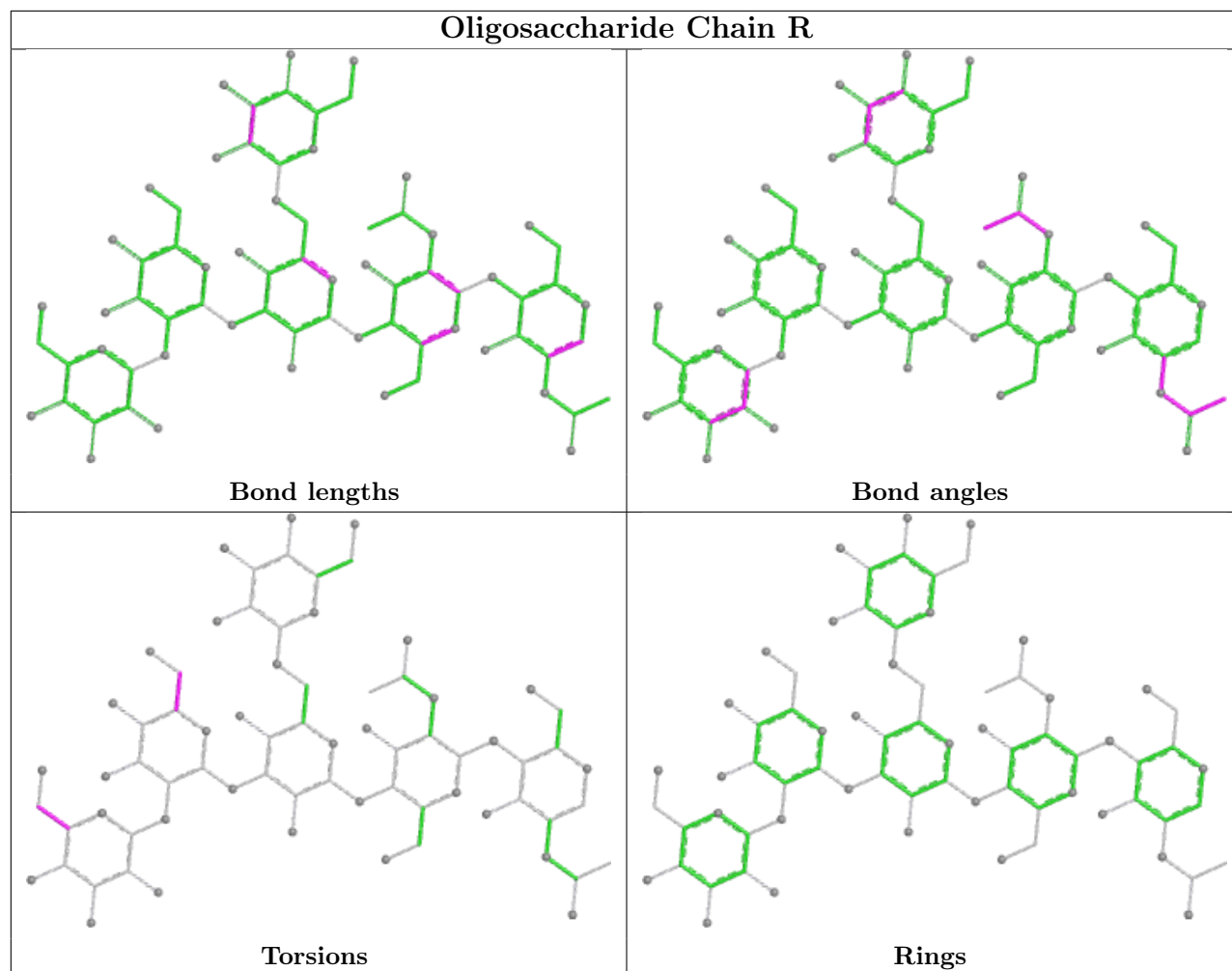


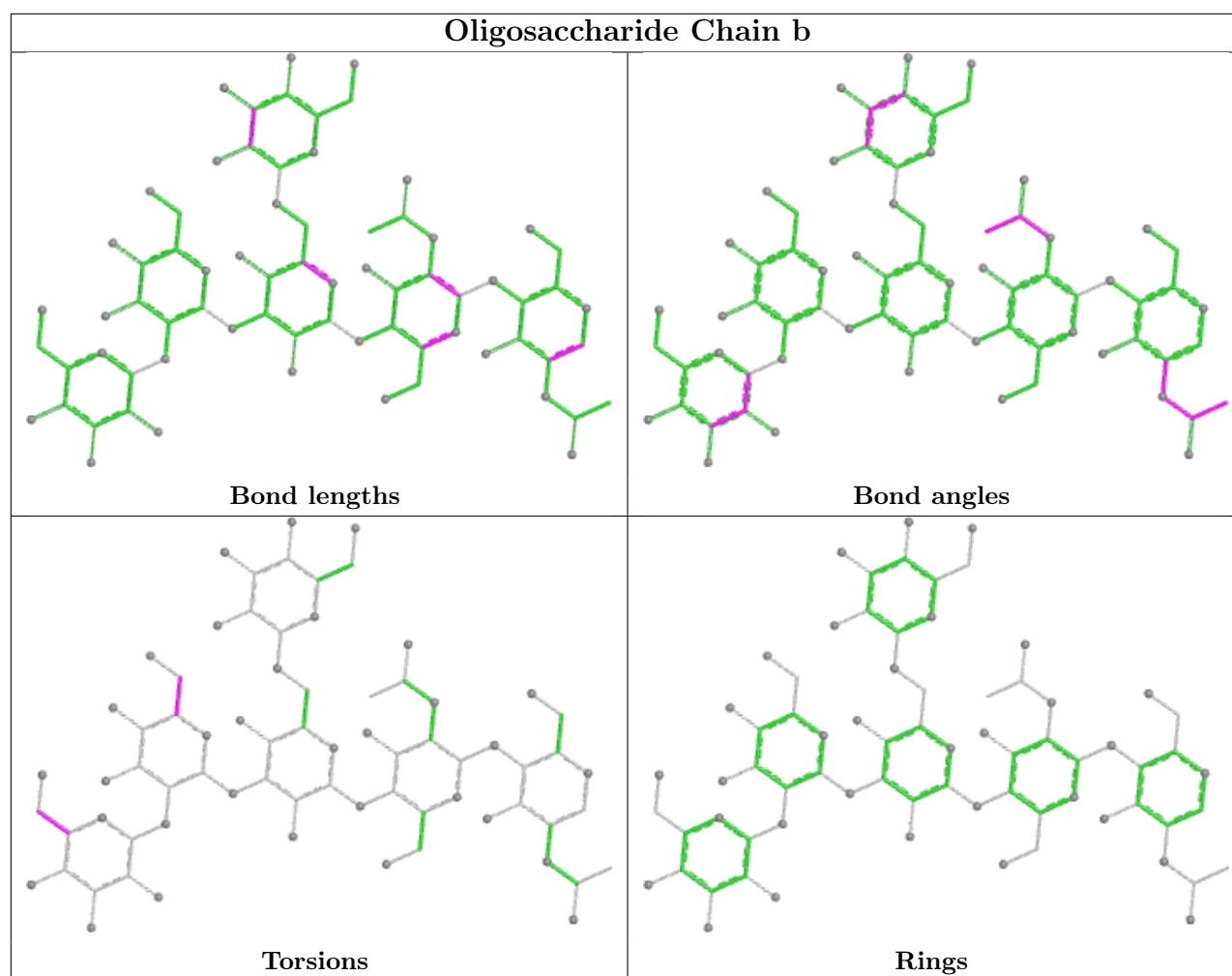












5.6 Ligand geometry [i](#)

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	1304	1	14,14,15	1.25	1 (7%)	17,19,21	1.07	1 (5%)
5	NAG	C	1303	1	14,14,15	1.22	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	C	1309	1	14,14,15	1.23	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	B	1301	1	14,14,15	1.25	1 (7%)	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1305	1	14,14,15	1.26	1 (7%)	17,19,21	1.13	1 (5%)
5	NAG	C	1306	1	14,14,15	1.26	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	B	1310	1	14,14,15	1.22	2 (14%)	17,19,21	1.10	1 (5%)
5	NAG	C	1301	1	14,14,15	1.25	1 (7%)	17,19,21	1.07	1 (5%)
5	NAG	A	1307	1	14,14,15	1.28	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	C	1307	1	14,14,15	1.29	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	A	1304	1	14,14,15	1.26	1 (7%)	17,19,21	1.07	1 (5%)
5	NAG	C	1302	1	14,14,15	1.47	2 (14%)	17,19,21	1.24	3 (17%)
5	NAG	C	1304	1	14,14,15	1.25	1 (7%)	17,19,21	1.07	1 (5%)
5	NAG	A	1301	1	14,14,15	1.25	1 (7%)	17,19,21	1.07	1 (5%)
5	NAG	B	1307	1	14,14,15	1.29	1 (7%)	17,19,21	1.06	1 (5%)
5	NAG	A	1308	1	14,14,15	1.35	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	A	1311	1	14,14,15	1.16	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	B	1306	1	14,14,15	1.26	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	C	1308	1	14,14,15	1.35	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	B	1305	1	14,14,15	1.25	2 (14%)	17,19,21	1.13	1 (5%)
5	NAG	B	1308	1	14,14,15	1.34	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	A	1310	1	14,14,15	1.23	2 (14%)	17,19,21	1.10	1 (5%)
5	NAG	B	1303	1	14,14,15	1.22	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	C	1310	1	14,14,15	1.23	2 (14%)	17,19,21	1.10	1 (5%)
5	NAG	A	1302	1	14,14,15	1.47	2 (14%)	17,19,21	1.23	3 (17%)
5	NAG	A	1309	1	14,14,15	1.23	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	A	1306	1	14,14,15	1.26	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	A	1305	1	14,14,15	1.26	1 (7%)	17,19,21	1.13	1 (5%)
5	NAG	B	1311	1	14,14,15	1.17	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	C	1311	1	14,14,15	1.16	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	A	1303	1	14,14,15	1.22	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	B	1302	1	14,14,15	1.48	2 (14%)	17,19,21	1.24	3 (17%)
5	NAG	B	1309	1	14,14,15	1.24	1 (7%)	17,19,21	1.08	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	B	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	0/6/23/26	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1308	NAG	C1-C2	4.02	1.57	1.52
5	A	1308	NAG	C1-C2	4.02	1.57	1.52
5	B	1308	NAG	C1-C2	3.99	1.57	1.52
5	B	1302	NAG	C1-C2	3.91	1.57	1.52
5	A	1302	NAG	C1-C2	3.90	1.57	1.52
5	C	1302	NAG	C1-C2	3.89	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1307	NAG	C1-C2	3.88	1.57	1.52
5	C	1307	NAG	C1-C2	3.83	1.57	1.52
5	A	1307	NAG	C1-C2	3.83	1.57	1.52
5	A	1305	NAG	C1-C2	3.77	1.57	1.52
5	C	1305	NAG	C1-C2	3.77	1.57	1.52
5	C	1306	NAG	C1-C2	3.76	1.57	1.52
5	A	1306	NAG	C1-C2	3.75	1.57	1.52
5	B	1306	NAG	C1-C2	3.75	1.57	1.52
5	B	1305	NAG	C1-C2	3.74	1.57	1.52
5	A	1304	NAG	C1-C2	3.68	1.57	1.52
5	B	1304	NAG	C1-C2	3.66	1.57	1.52
5	C	1304	NAG	C1-C2	3.65	1.57	1.52
5	B	1309	NAG	C1-C2	3.63	1.57	1.52
5	A	1309	NAG	C1-C2	3.61	1.57	1.52
5	B	1301	NAG	C1-C2	3.61	1.57	1.52
5	C	1309	NAG	C1-C2	3.61	1.57	1.52
5	C	1301	NAG	C1-C2	3.61	1.57	1.52
5	A	1301	NAG	C1-C2	3.60	1.57	1.52
5	A	1303	NAG	C1-C2	3.55	1.57	1.52
5	C	1303	NAG	C1-C2	3.53	1.57	1.52
5	B	1303	NAG	C1-C2	3.52	1.57	1.52
5	C	1310	NAG	C1-C2	3.42	1.57	1.52
5	A	1310	NAG	C1-C2	3.41	1.57	1.52
5	B	1311	NAG	C1-C2	3.40	1.57	1.52
5	B	1310	NAG	C1-C2	3.38	1.56	1.52
5	A	1311	NAG	C1-C2	3.36	1.56	1.52
5	C	1311	NAG	C1-C2	3.32	1.56	1.52
5	B	1302	NAG	O5-C5	2.21	1.47	1.43
5	A	1310	NAG	O5-C5	2.20	1.47	1.43
5	C	1310	NAG	O5-C5	2.19	1.47	1.43
5	B	1310	NAG	O5-C5	2.19	1.47	1.43
5	A	1302	NAG	O5-C5	2.17	1.47	1.43
5	C	1302	NAG	O5-C5	2.16	1.47	1.43
5	B	1305	NAG	O5-C5	2.00	1.47	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1305	NAG	C8-C7-N2	2.59	120.42	116.12
5	A	1305	NAG	C8-C7-N2	2.59	120.41	116.12
5	C	1305	NAG	C8-C7-N2	2.59	120.41	116.12
5	B	1307	NAG	C8-C7-N2	2.58	120.39	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1307	NAG	C8-C7-N2	2.57	120.38	116.12
5	A	1307	NAG	C8-C7-N2	2.57	120.37	116.12
5	B	1306	NAG	C8-C7-N2	2.54	120.33	116.12
5	A	1306	NAG	C8-C7-N2	2.54	120.33	116.12
5	C	1301	NAG	C8-C7-N2	2.54	120.32	116.12
5	C	1306	NAG	C8-C7-N2	2.53	120.32	116.12
5	B	1301	NAG	C8-C7-N2	2.53	120.31	116.12
5	A	1301	NAG	C8-C7-N2	2.52	120.30	116.12
5	A	1309	NAG	C8-C7-N2	2.50	120.27	116.12
5	C	1309	NAG	C8-C7-N2	2.49	120.25	116.12
5	B	1302	NAG	C4-C3-C2	-2.49	107.38	111.02
5	B	1309	NAG	C8-C7-N2	2.48	120.23	116.12
5	C	1302	NAG	C4-C3-C2	-2.48	107.38	111.02
5	A	1302	NAG	C4-C3-C2	-2.48	107.38	111.02
5	B	1308	NAG	C8-C7-N2	2.44	120.17	116.12
5	C	1308	NAG	C8-C7-N2	2.44	120.17	116.12
5	A	1308	NAG	C8-C7-N2	2.44	120.16	116.12
5	C	1303	NAG	C8-C7-N2	2.43	120.15	116.12
5	A	1304	NAG	C8-C7-N2	2.43	120.14	116.12
5	C	1304	NAG	C8-C7-N2	2.42	120.14	116.12
5	C	1311	NAG	C8-C7-N2	2.42	120.14	116.12
5	A	1311	NAG	C8-C7-N2	2.42	120.13	116.12
5	B	1304	NAG	C8-C7-N2	2.41	120.12	116.12
5	B	1311	NAG	C8-C7-N2	2.41	120.12	116.12
5	A	1303	NAG	C8-C7-N2	2.40	120.11	116.12
5	C	1302	NAG	C8-C7-N2	2.40	120.10	116.12
5	B	1303	NAG	C8-C7-N2	2.40	120.09	116.12
5	B	1302	NAG	C8-C7-N2	2.38	120.06	116.12
5	A	1302	NAG	C8-C7-N2	2.38	120.06	116.12
5	B	1310	NAG	C8-C7-N2	2.32	119.97	116.12
5	A	1310	NAG	C8-C7-N2	2.32	119.97	116.12
5	C	1310	NAG	C8-C7-N2	2.31	119.95	116.12
5	B	1302	NAG	C2-N2-C7	-2.10	120.09	122.90
5	A	1302	NAG	C2-N2-C7	-2.09	120.09	122.90
5	C	1302	NAG	C2-N2-C7	-2.07	120.12	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1301	NAG	C4-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6

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Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1301	NAG	C4-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6

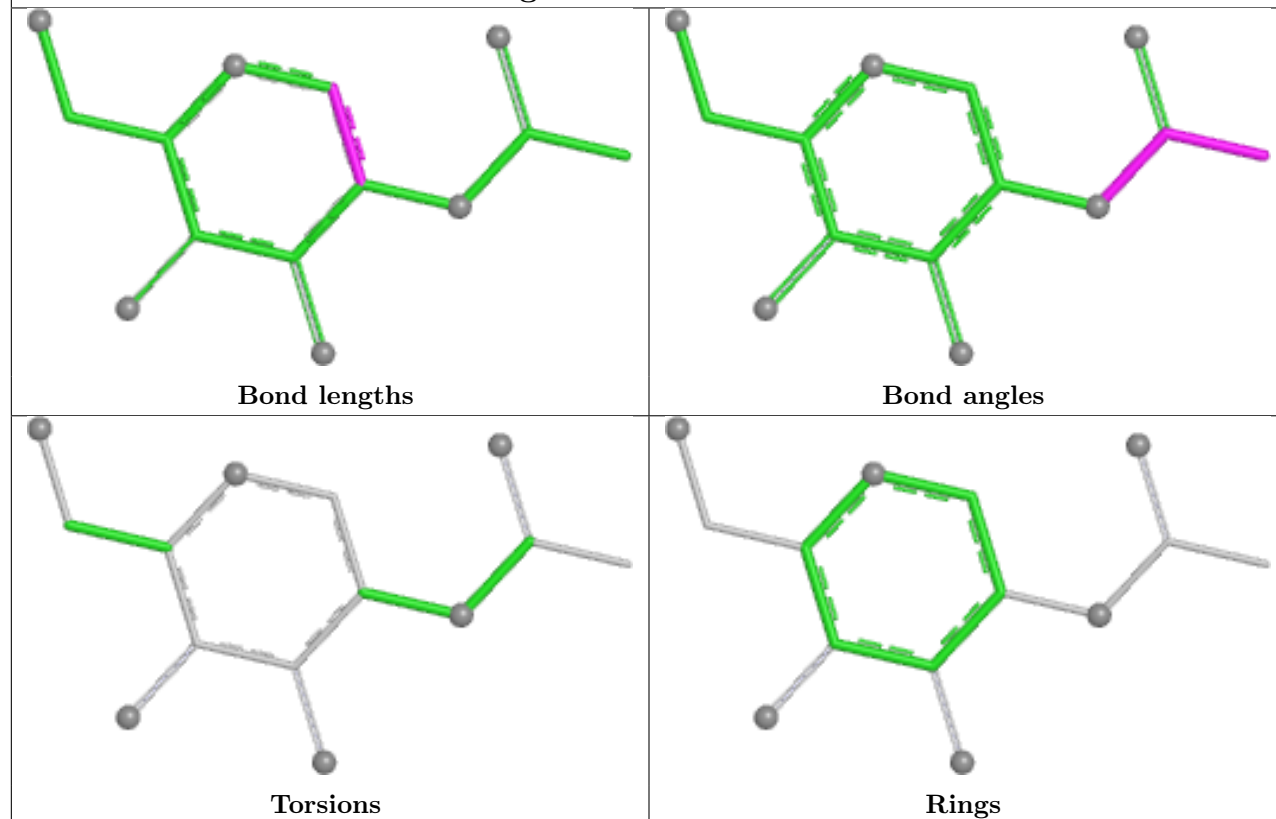
There are no ring outliers.

3 monomers are involved in 8 short contacts:

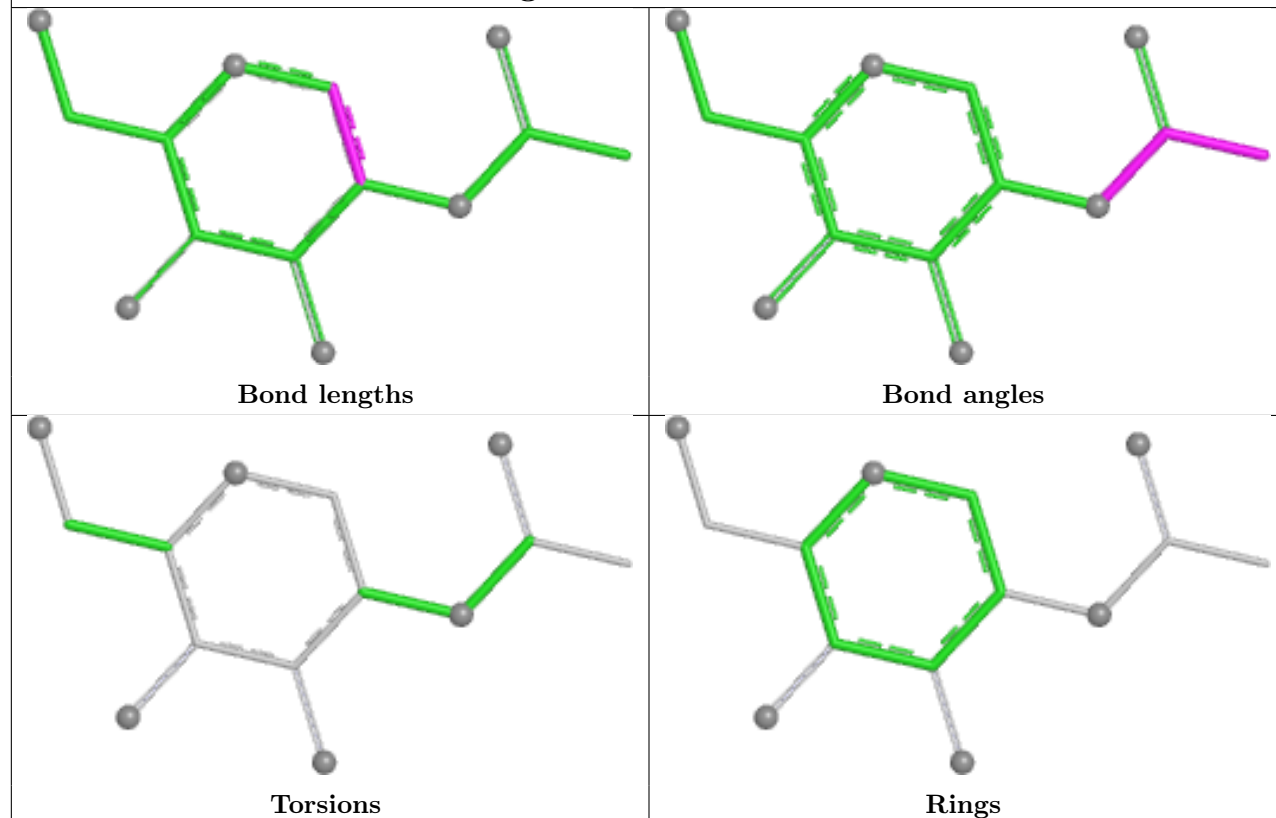
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1305	NAG	2	0
5	B	1305	NAG	3	0
5	A	1305	NAG	3	0

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.

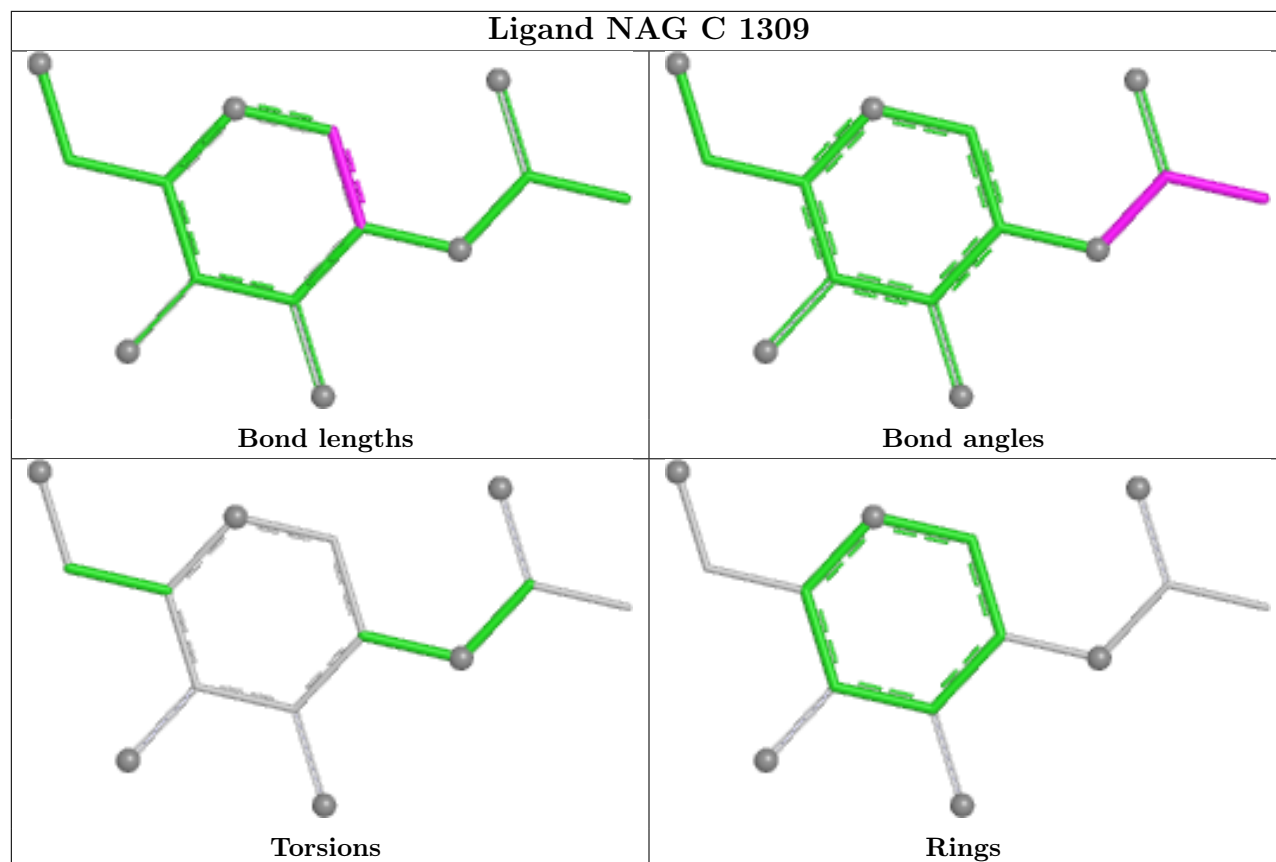
Ligand NAG B 1304



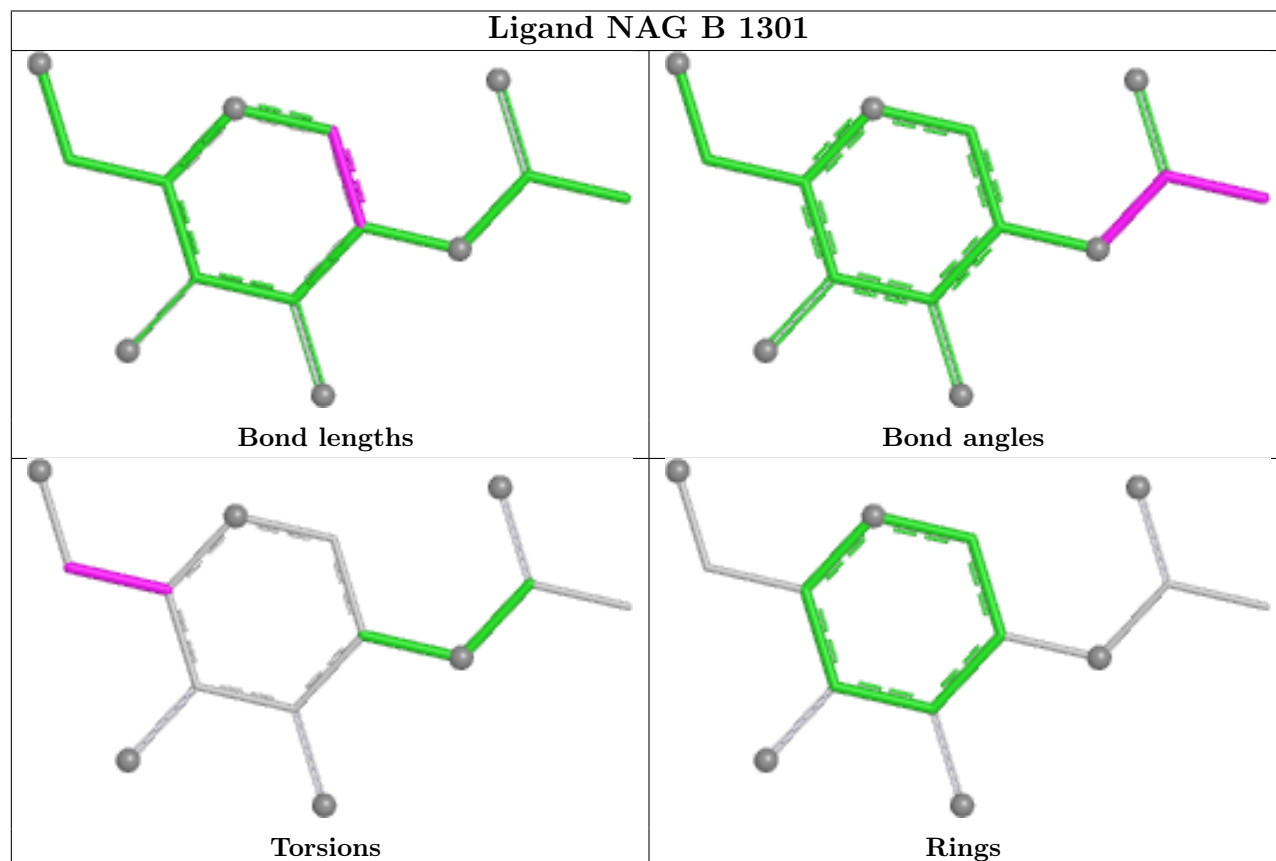
Ligand NAG C 1303

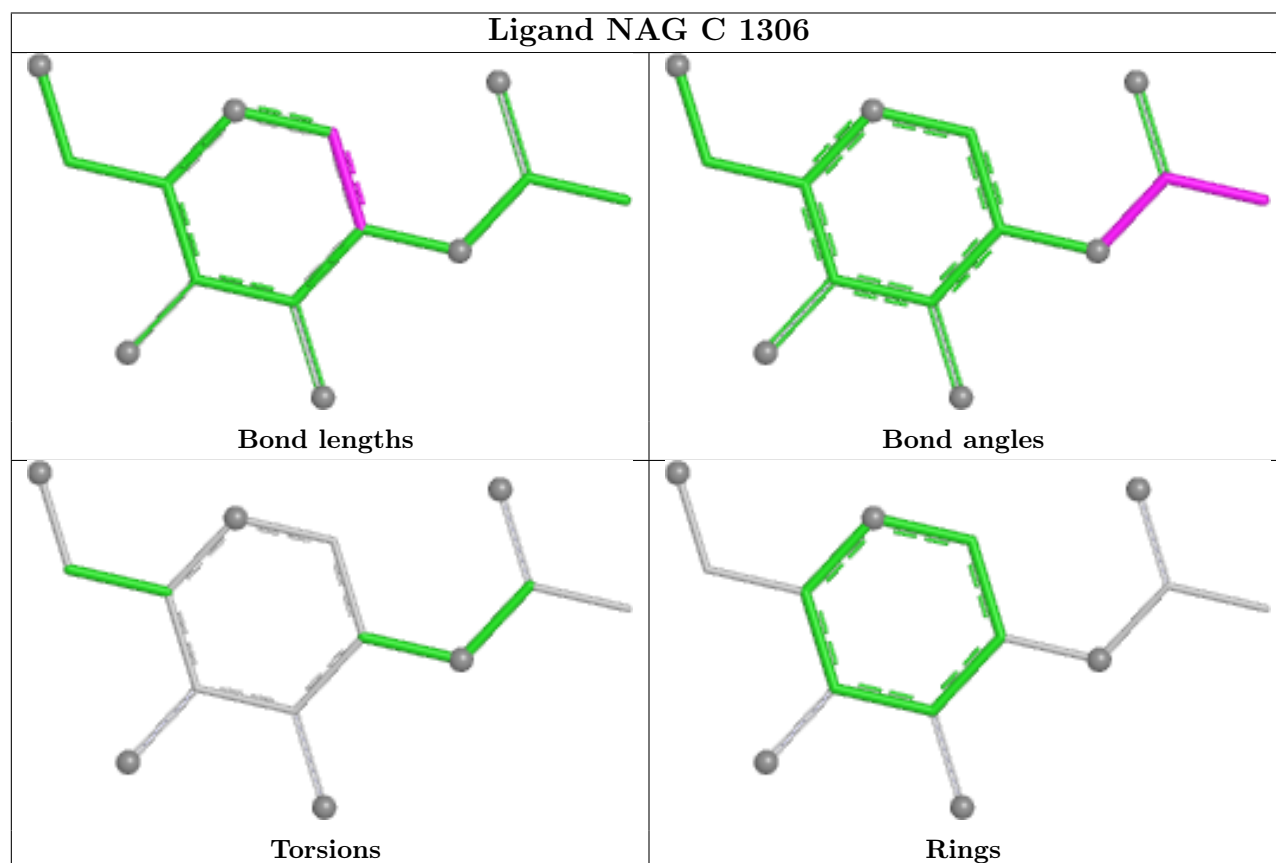
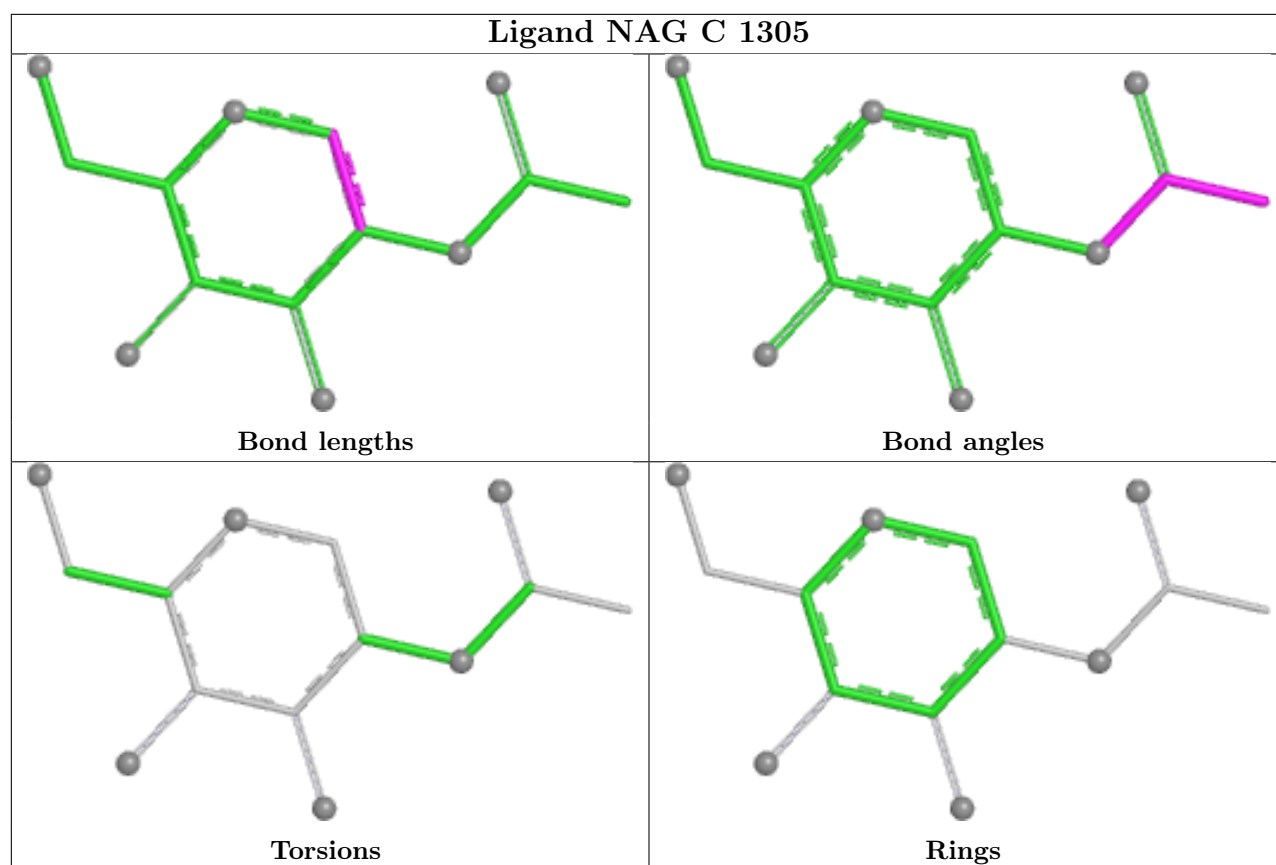


Ligand NAG C 1309

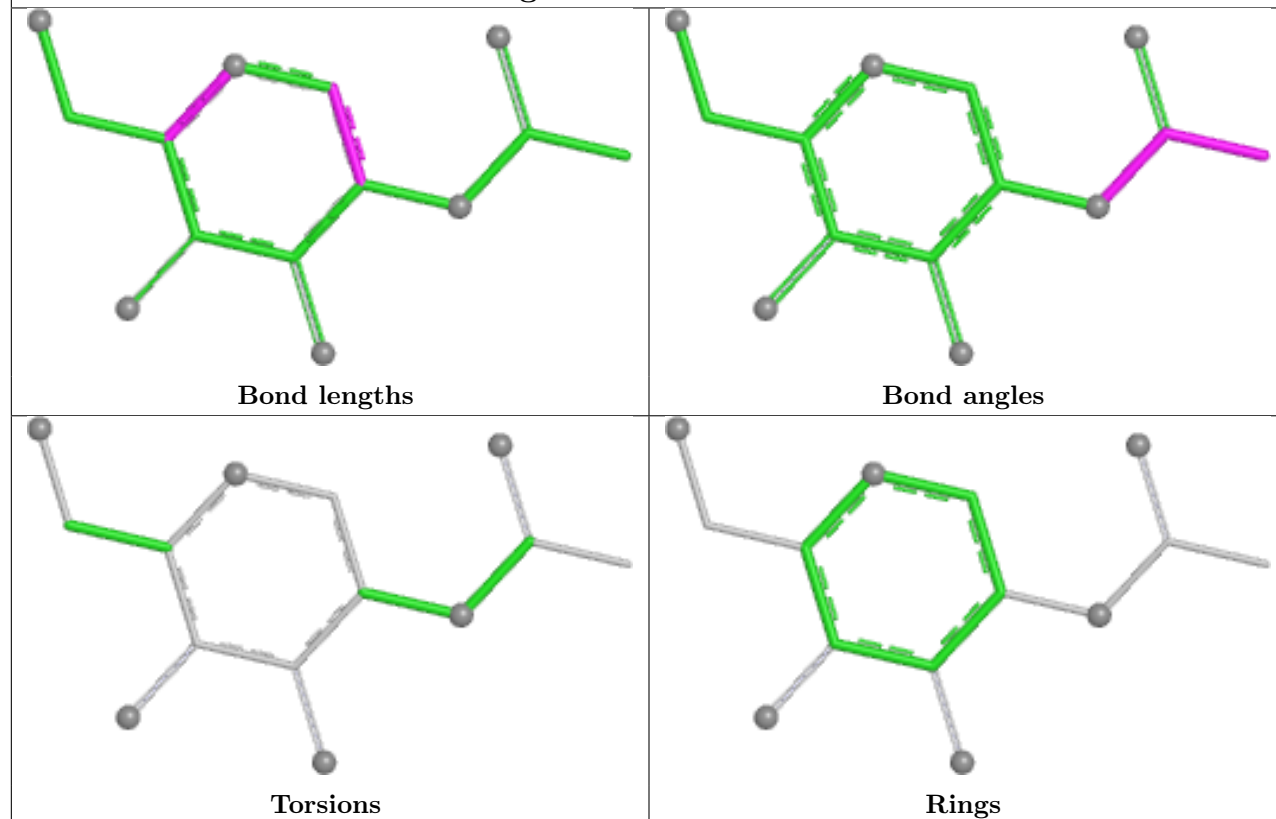


Ligand NAG B 1301

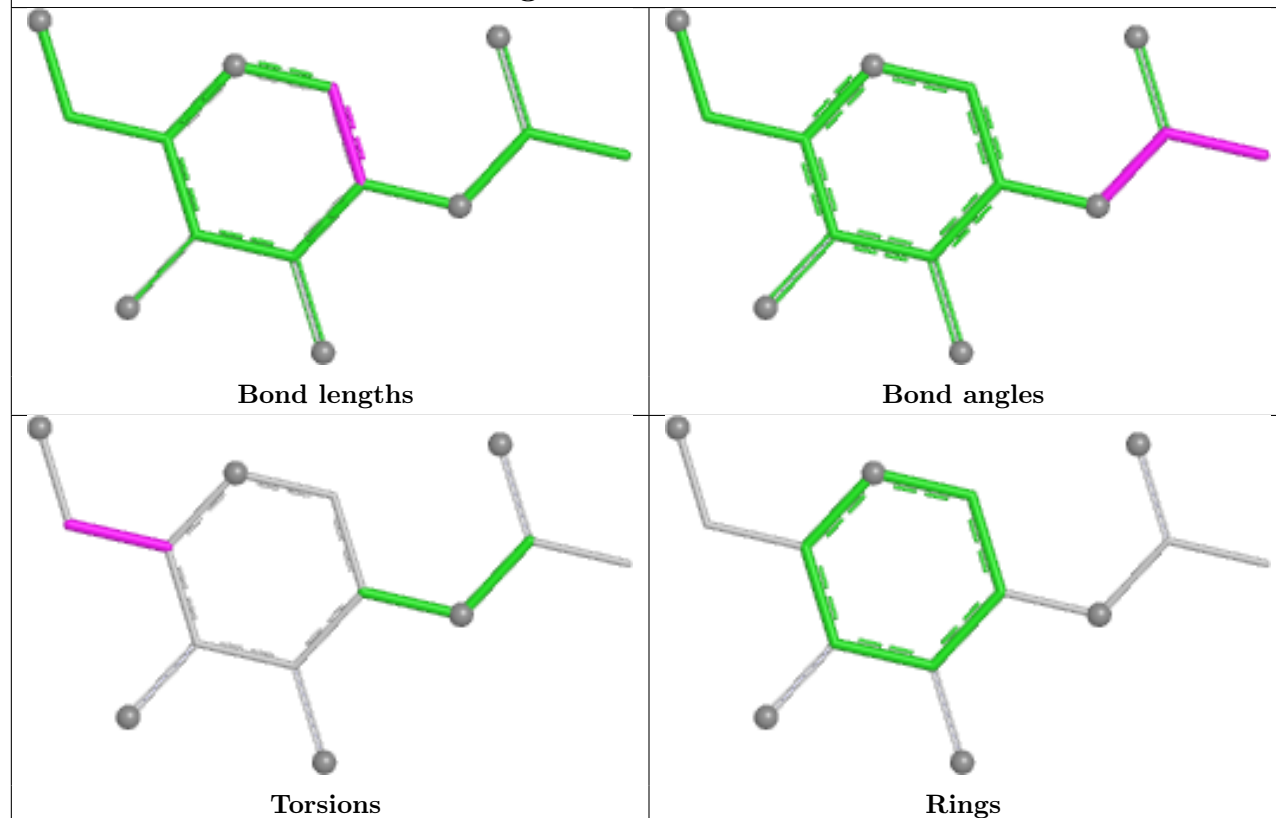


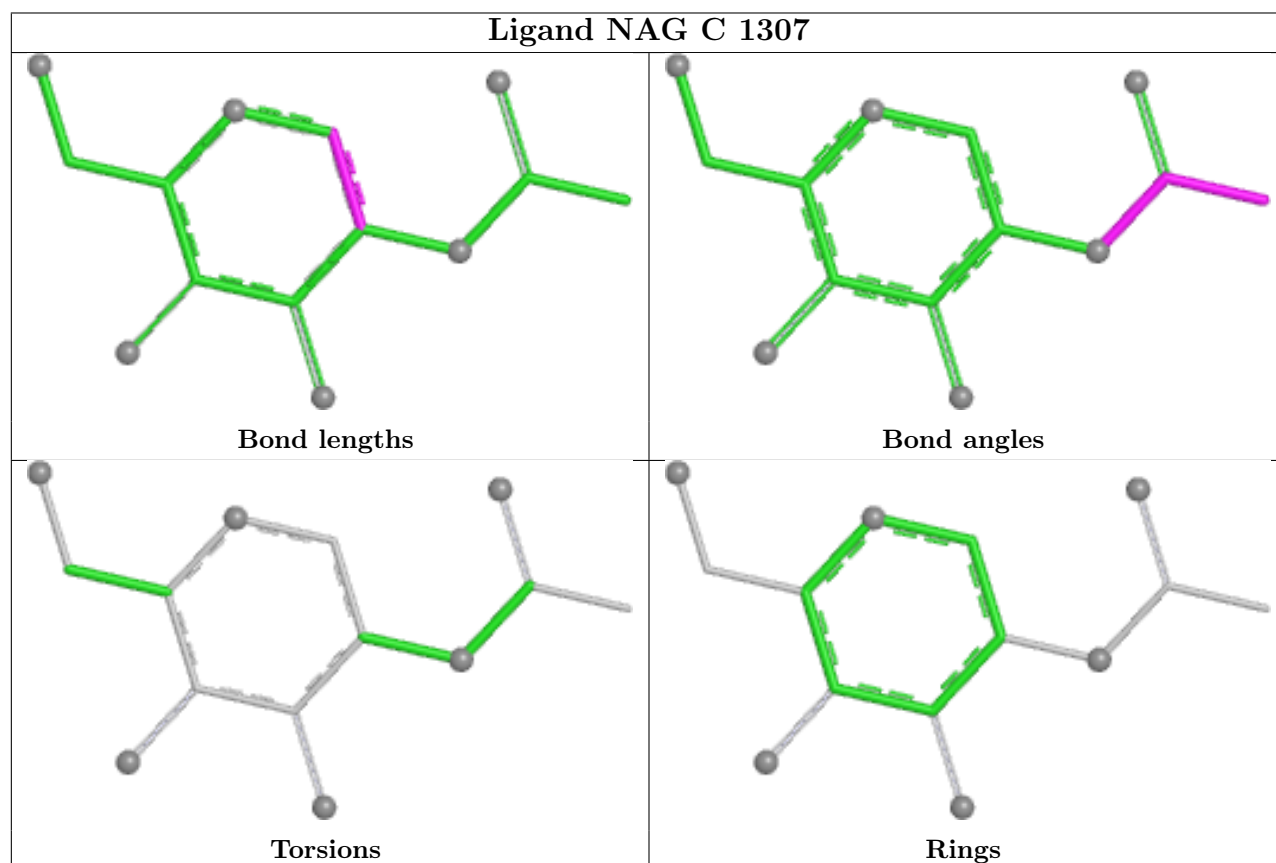
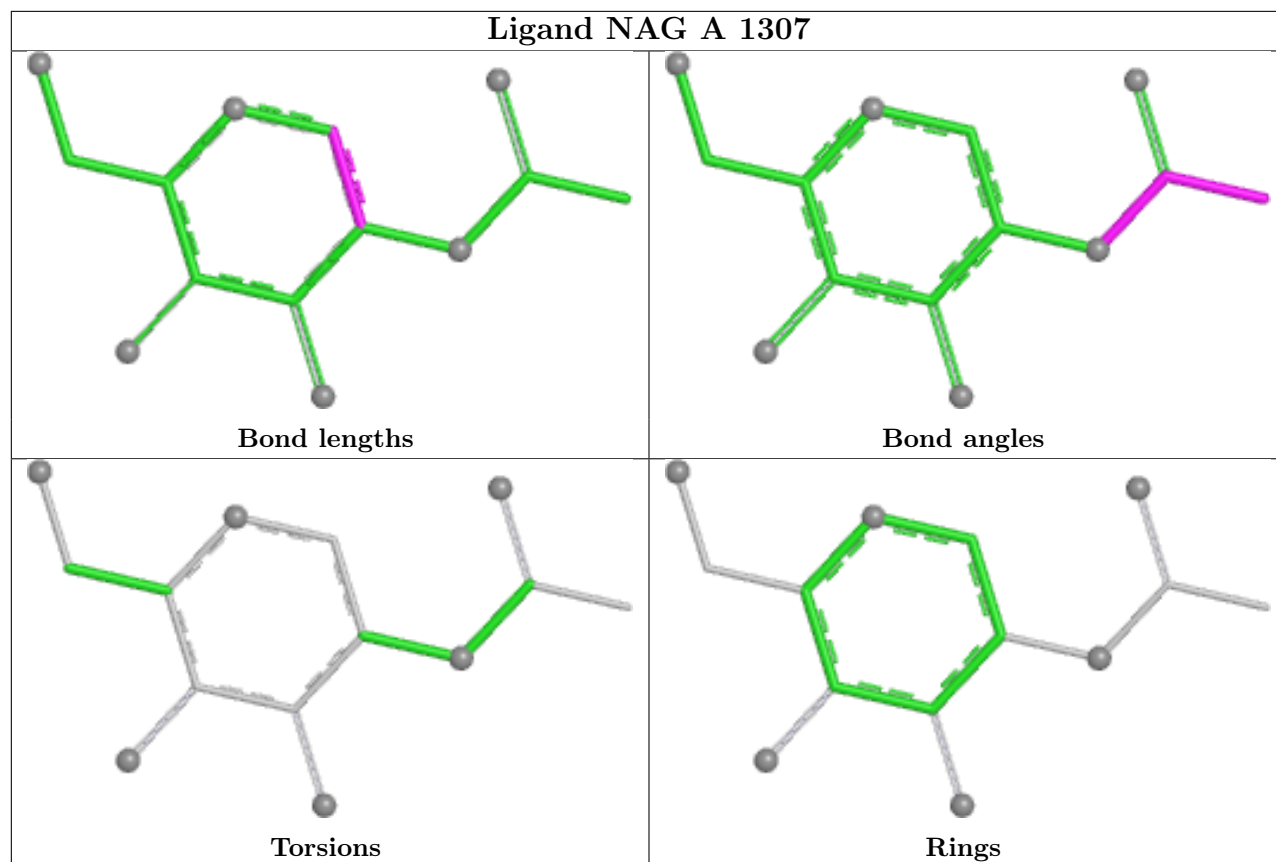


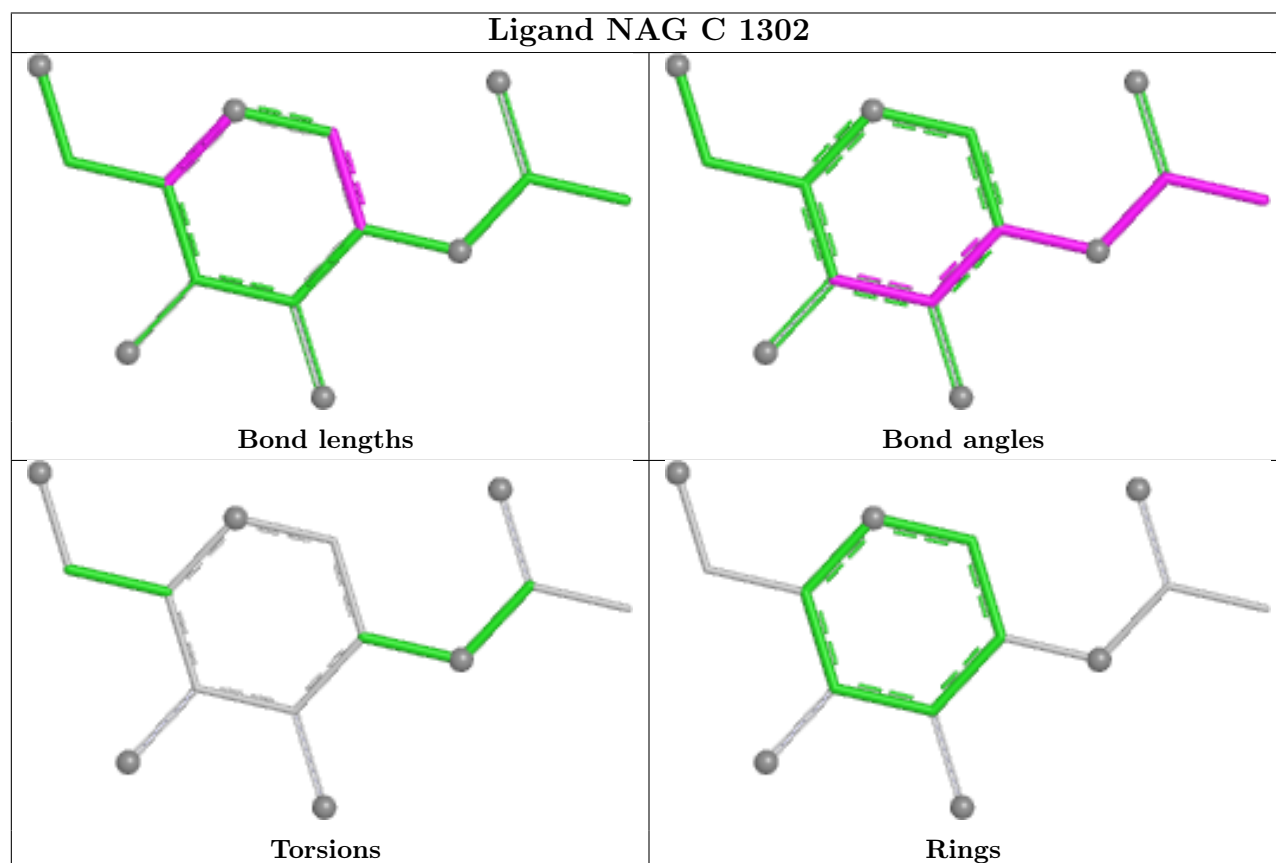
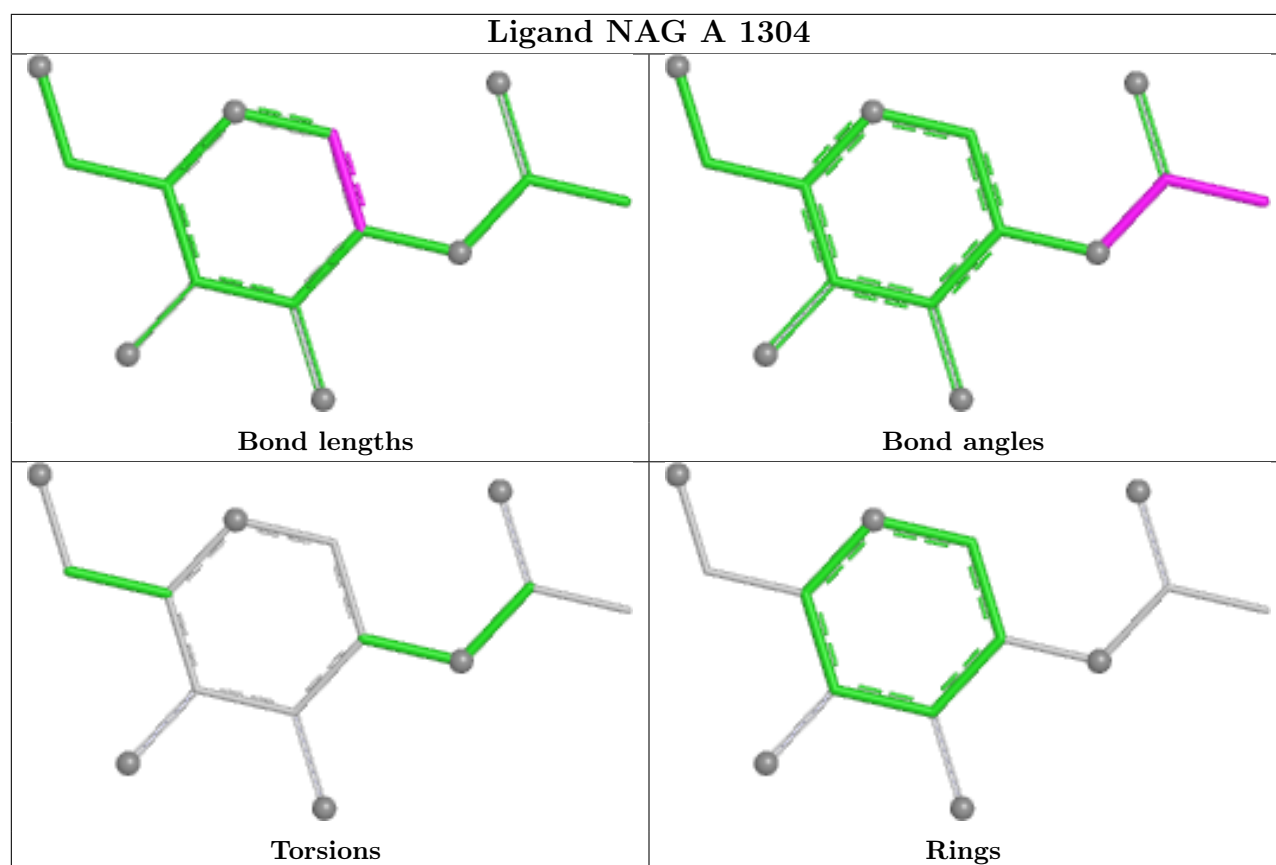
Ligand NAG B 1310

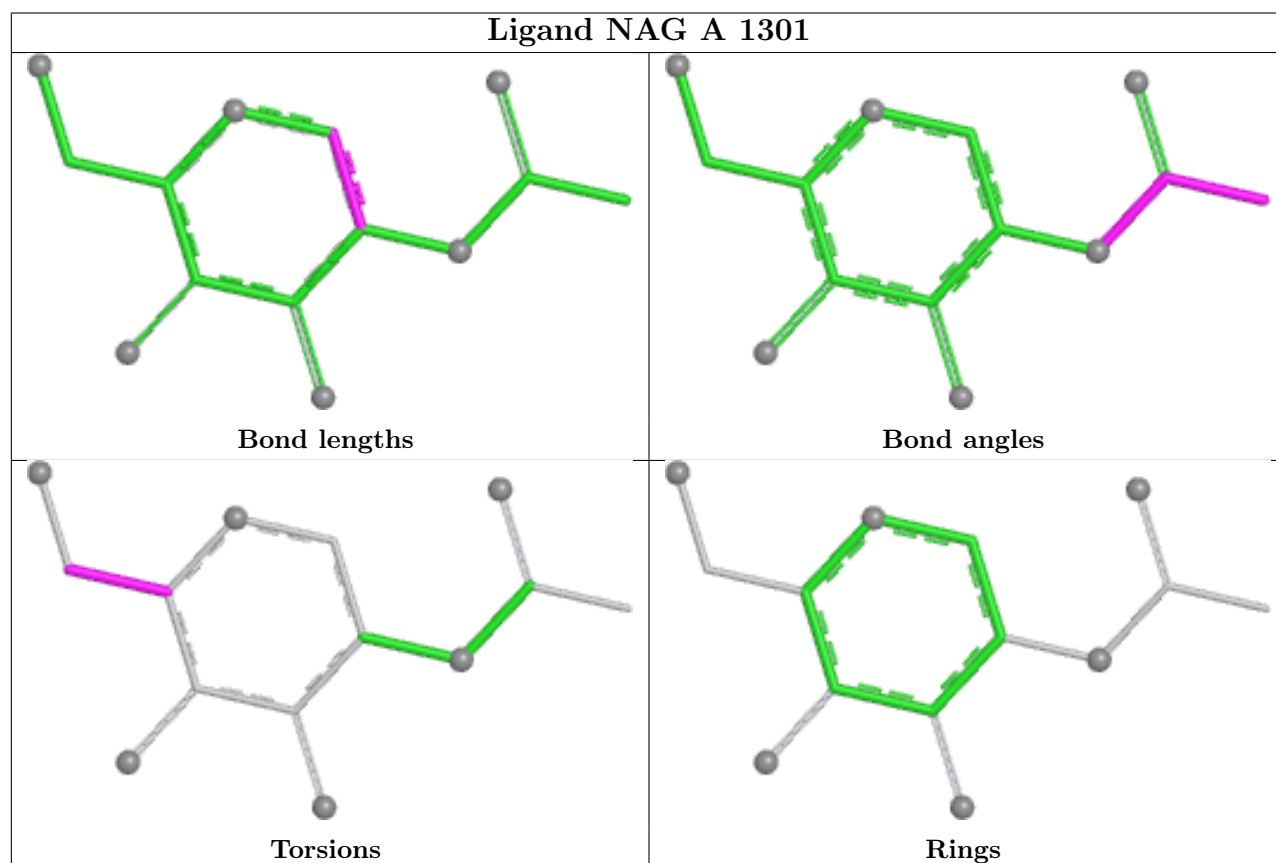
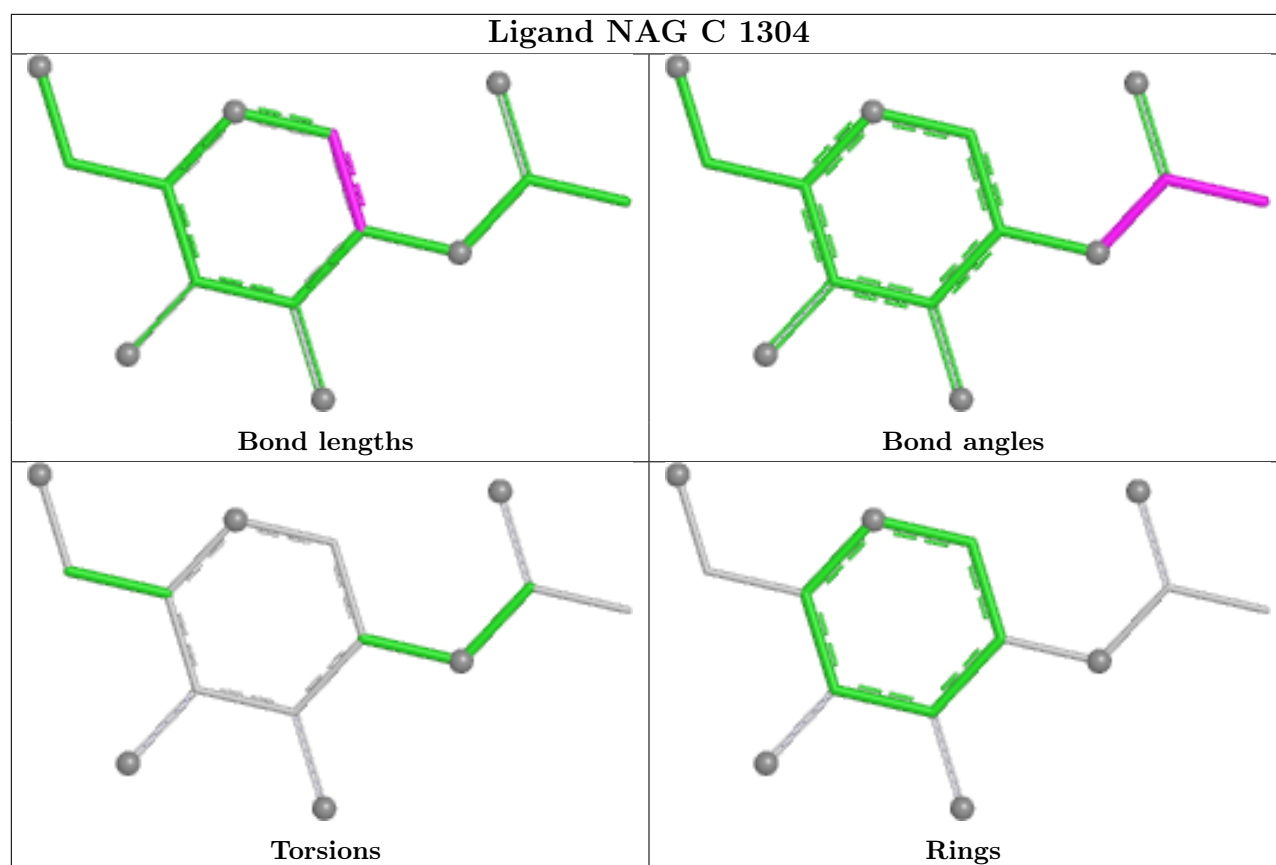


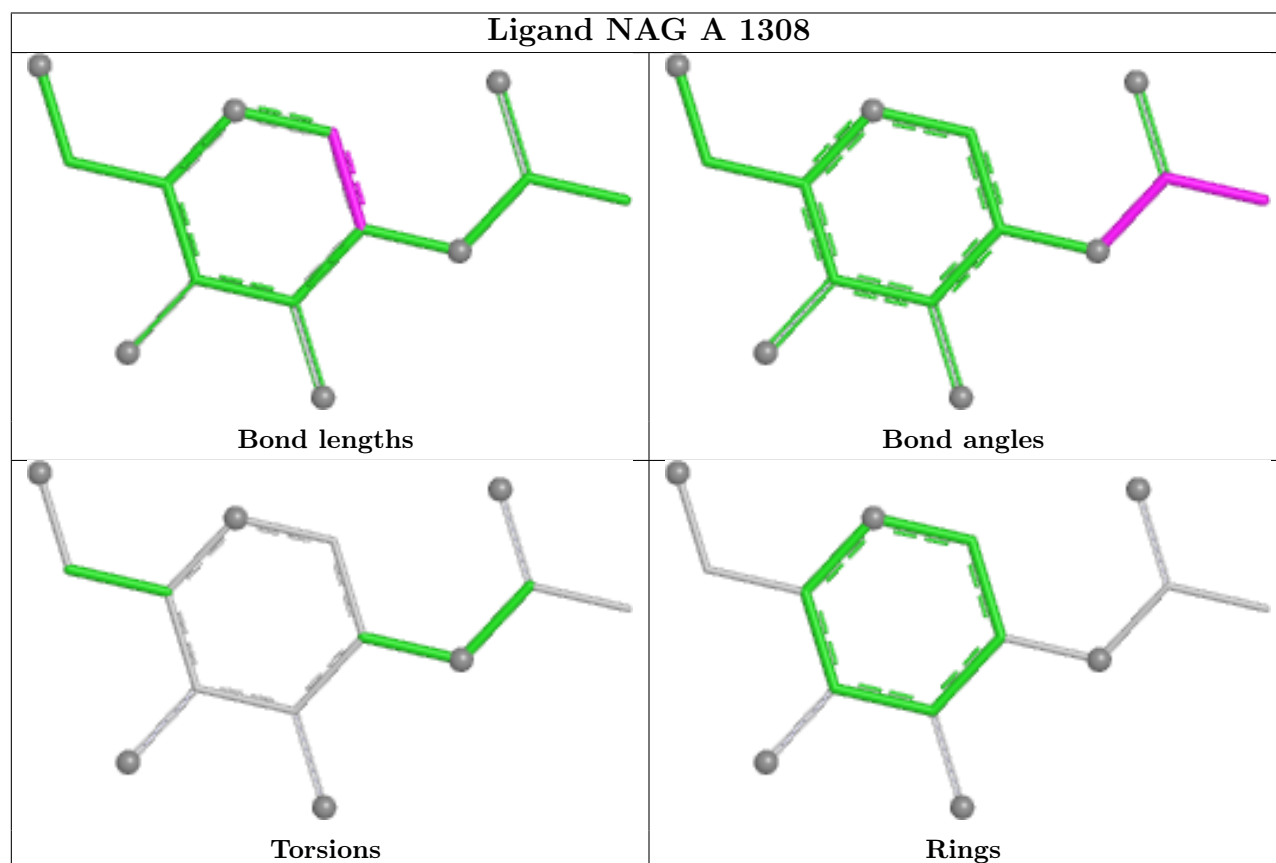
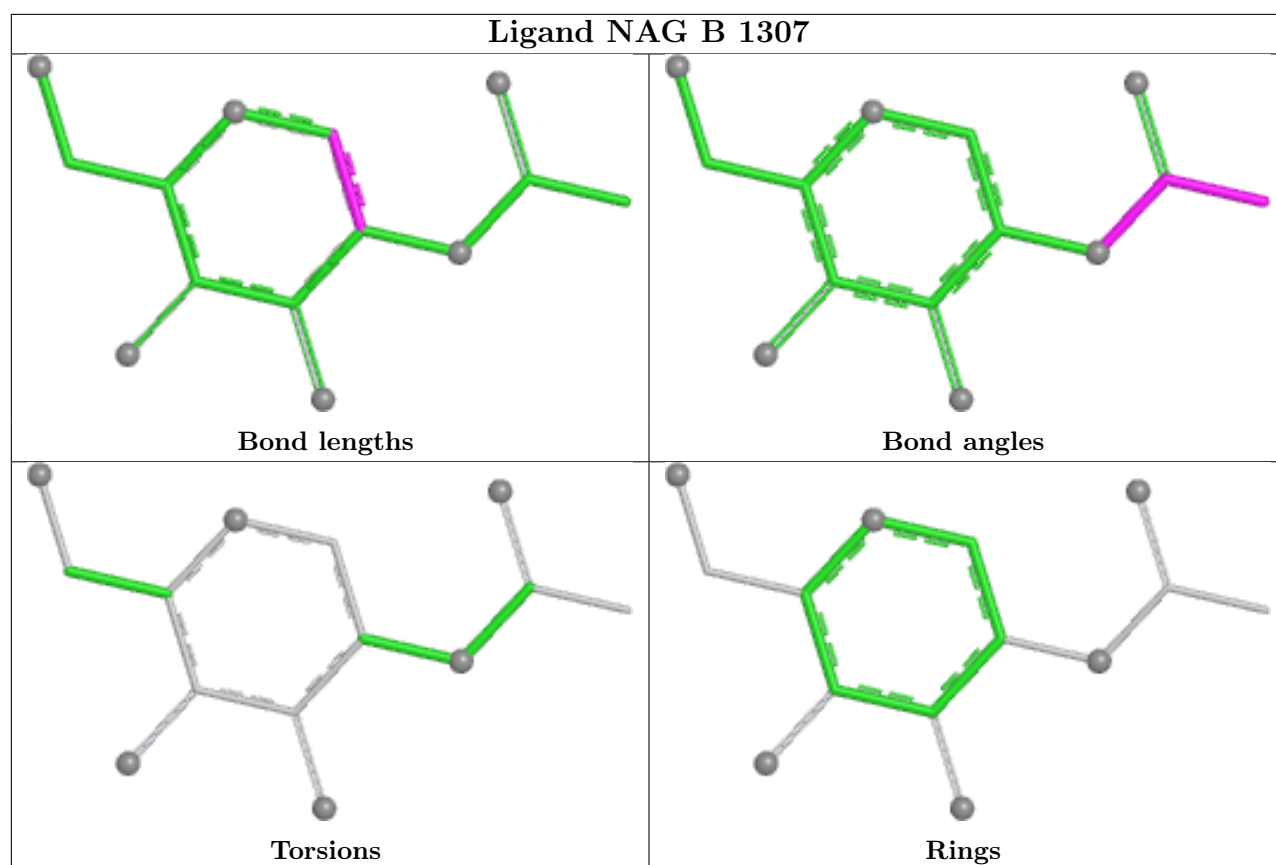
Ligand NAG C 1301

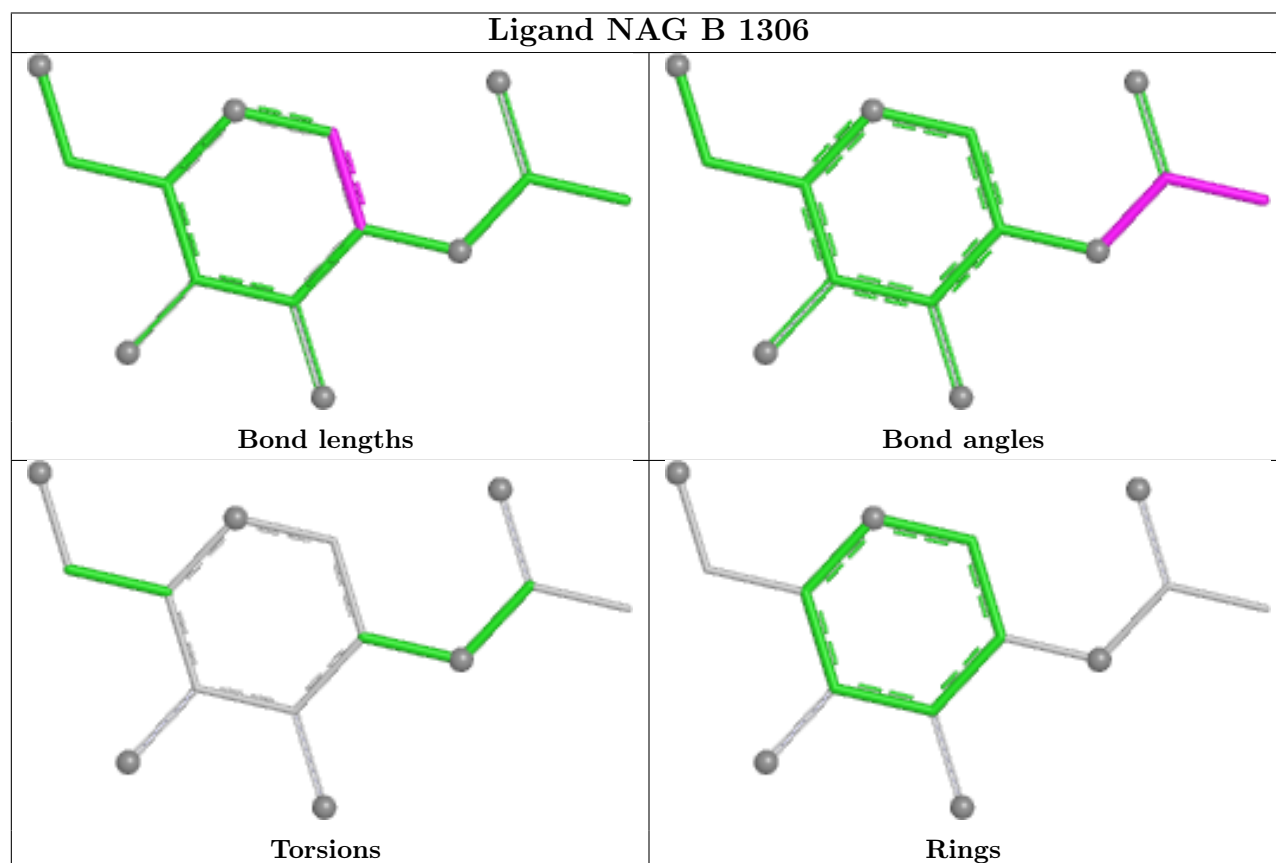
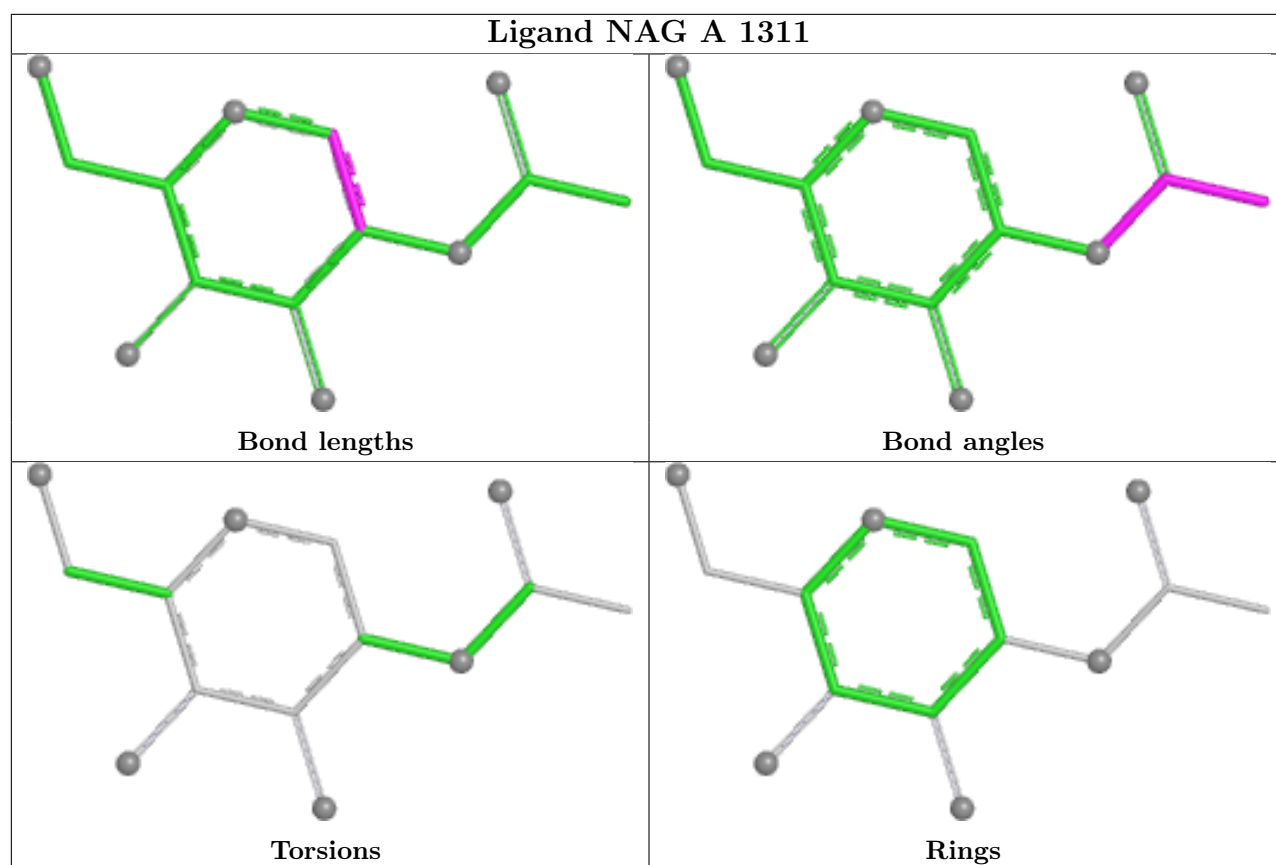


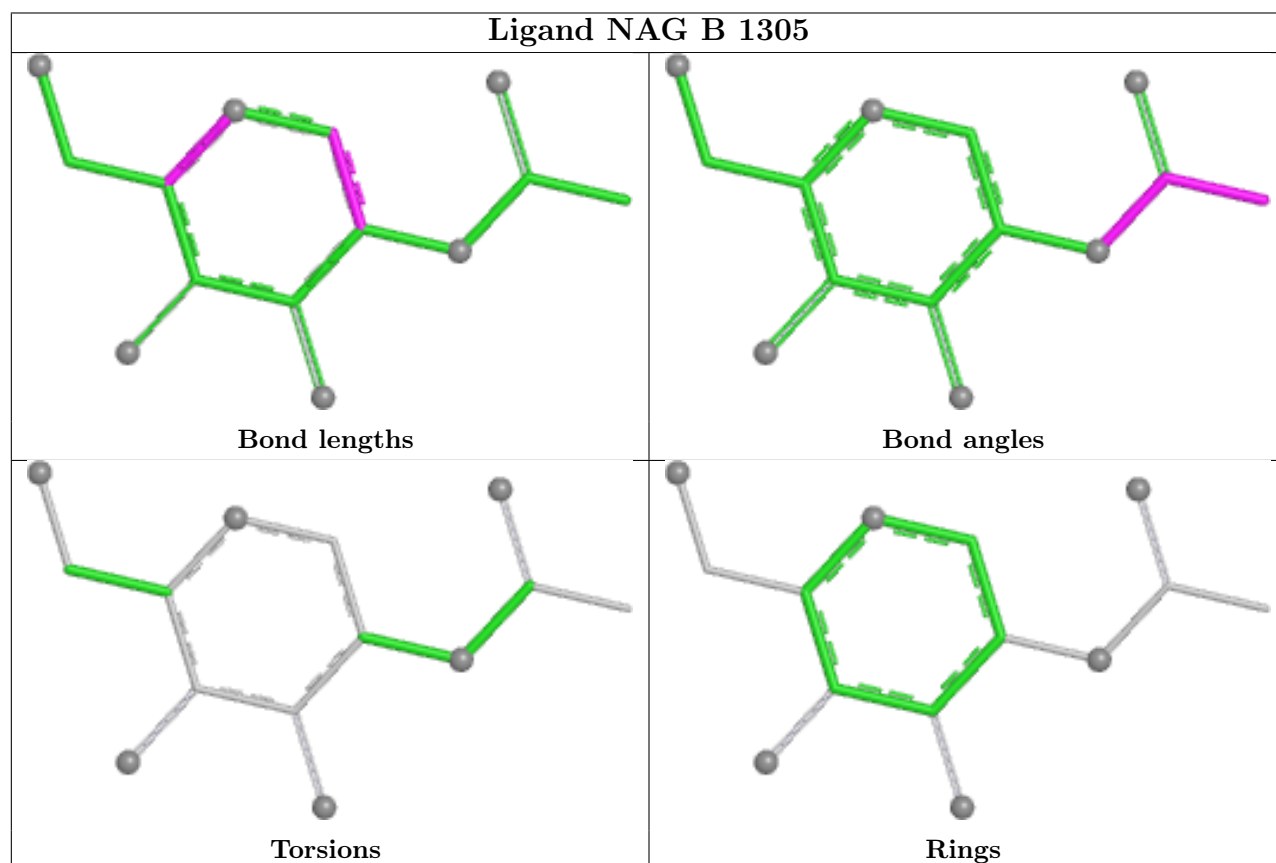
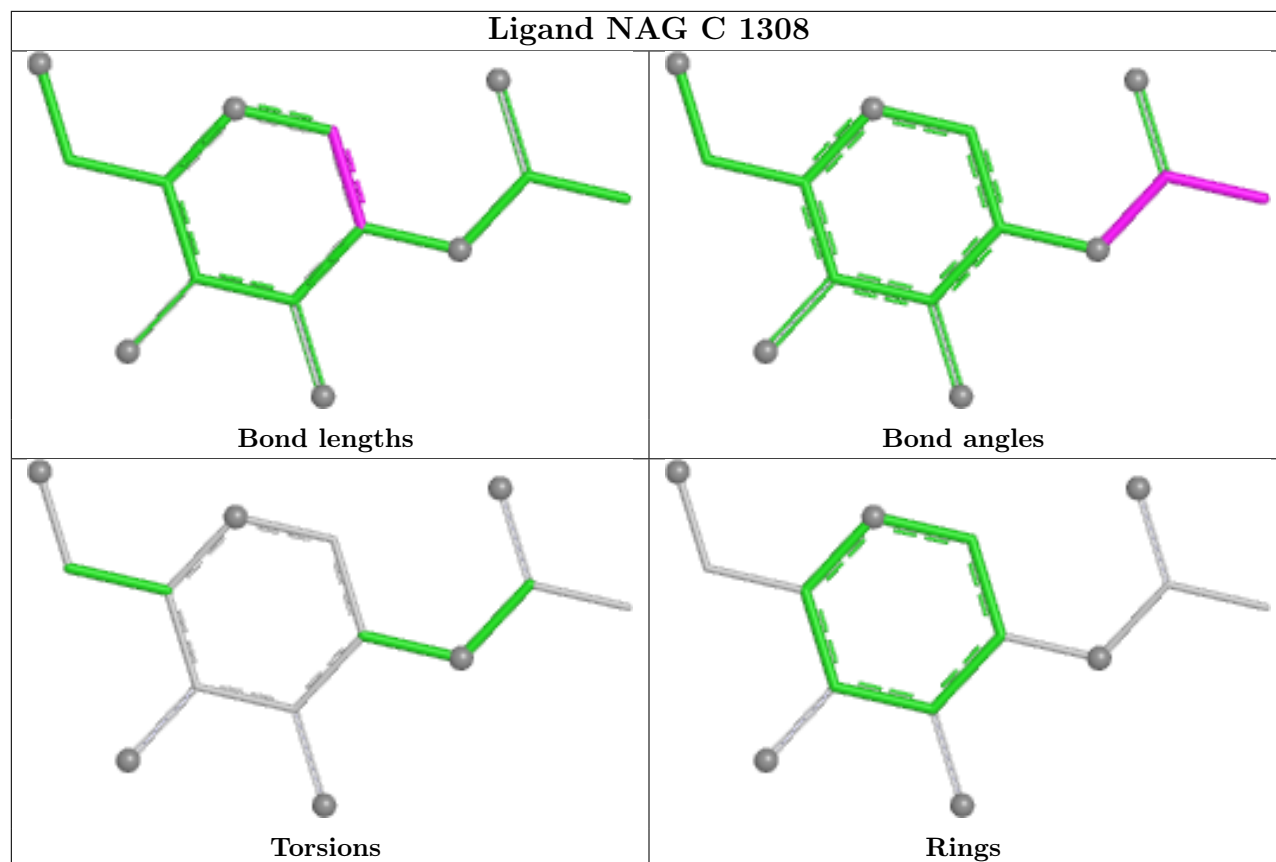




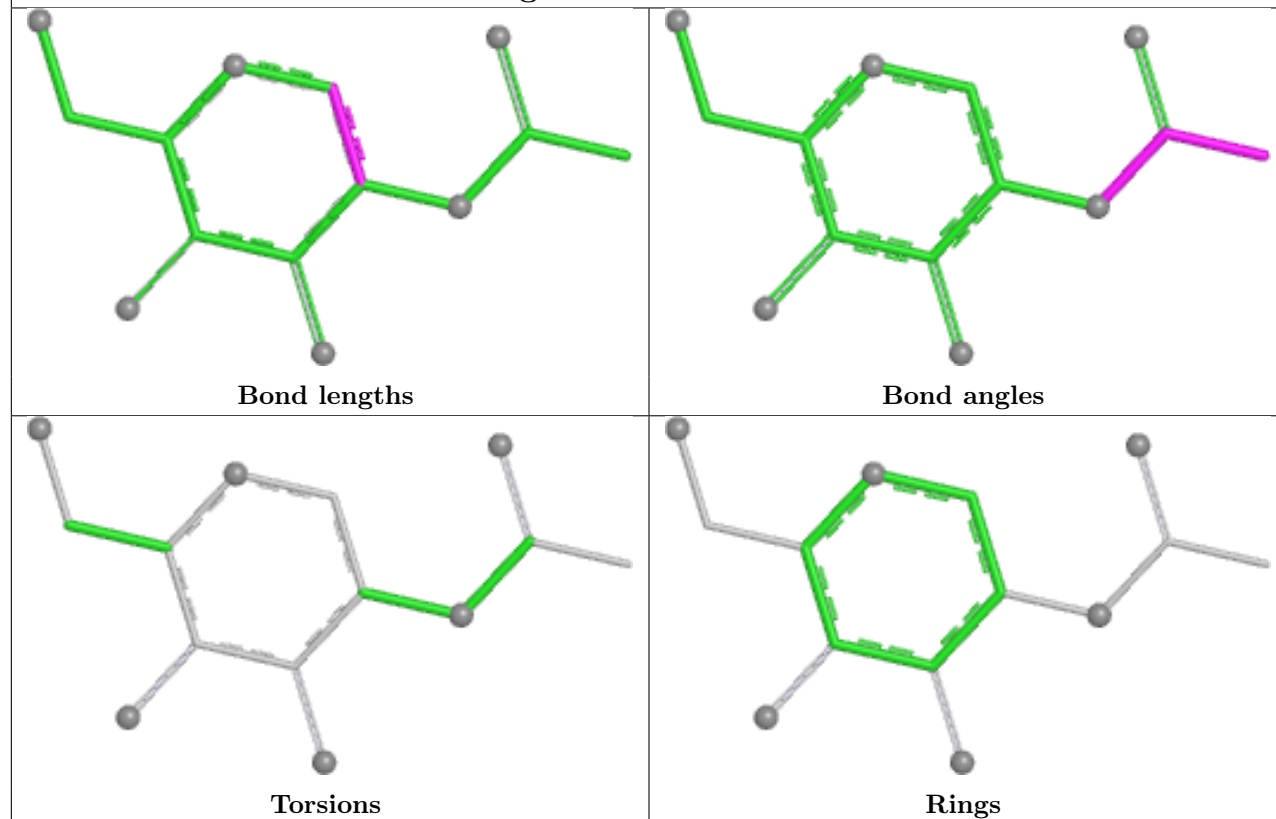




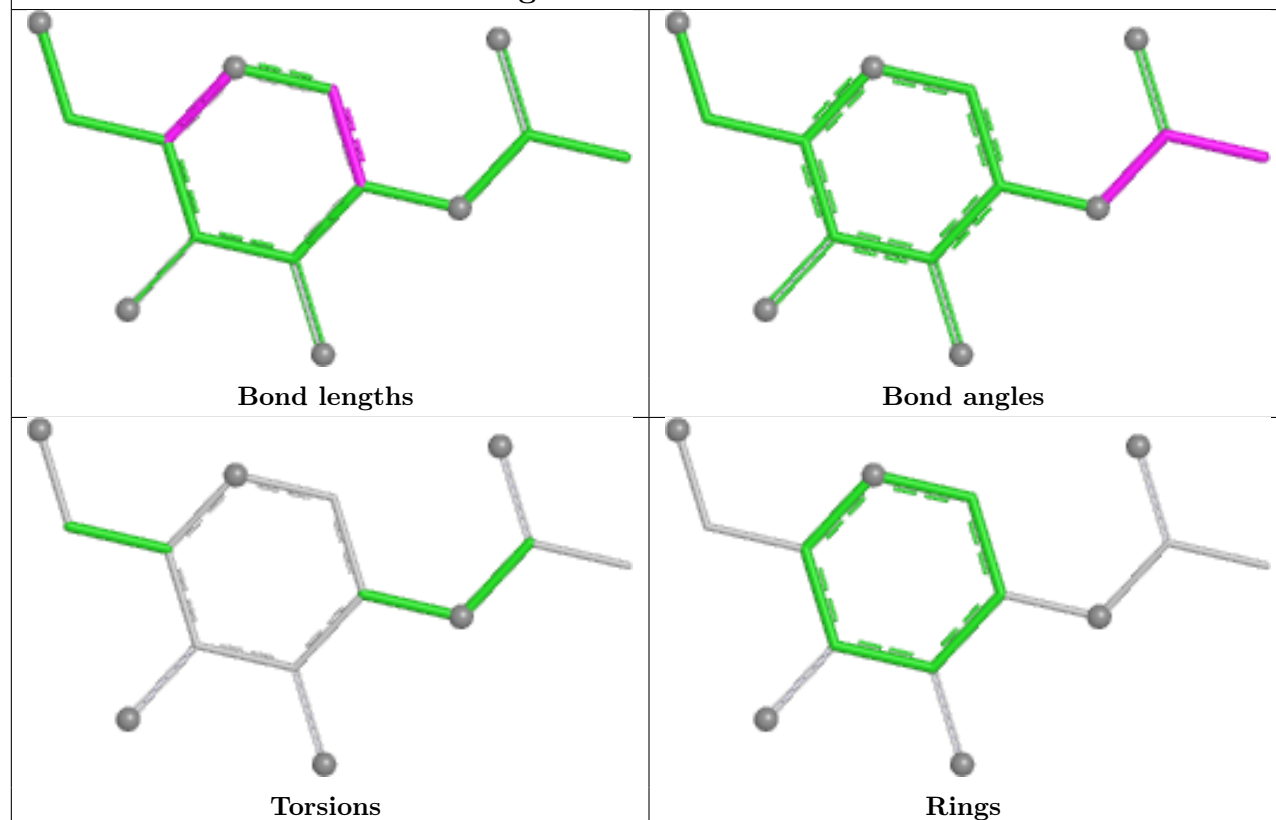




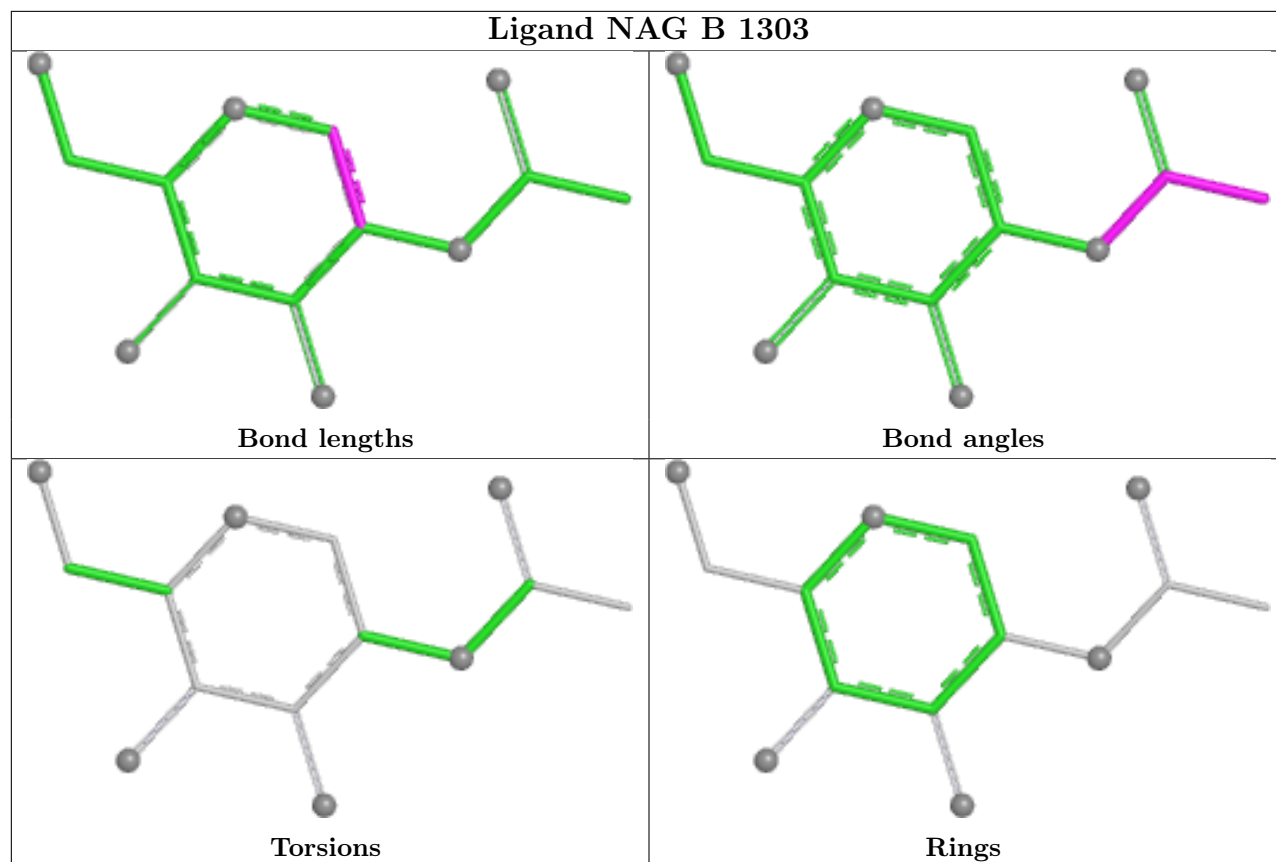
Ligand NAG B 1308



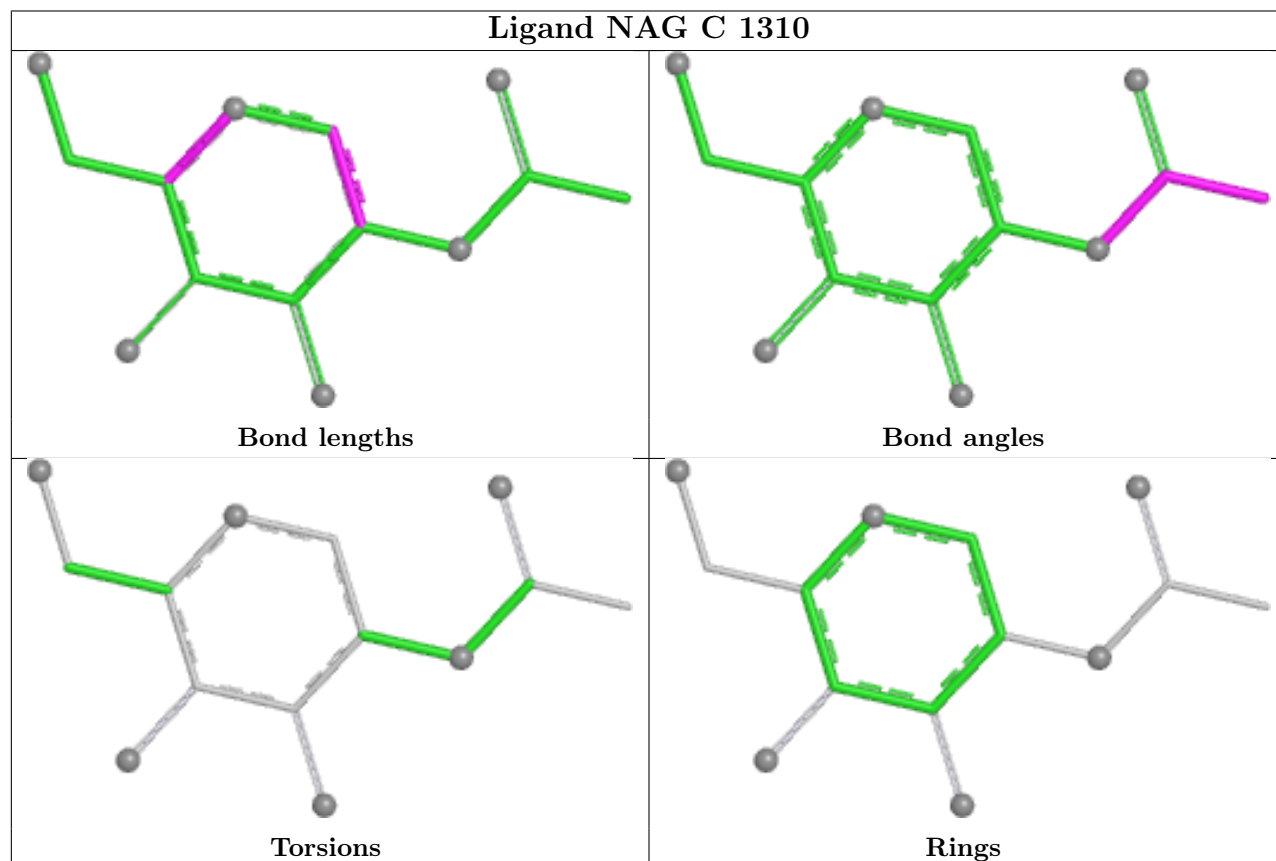
Ligand NAG A 1310

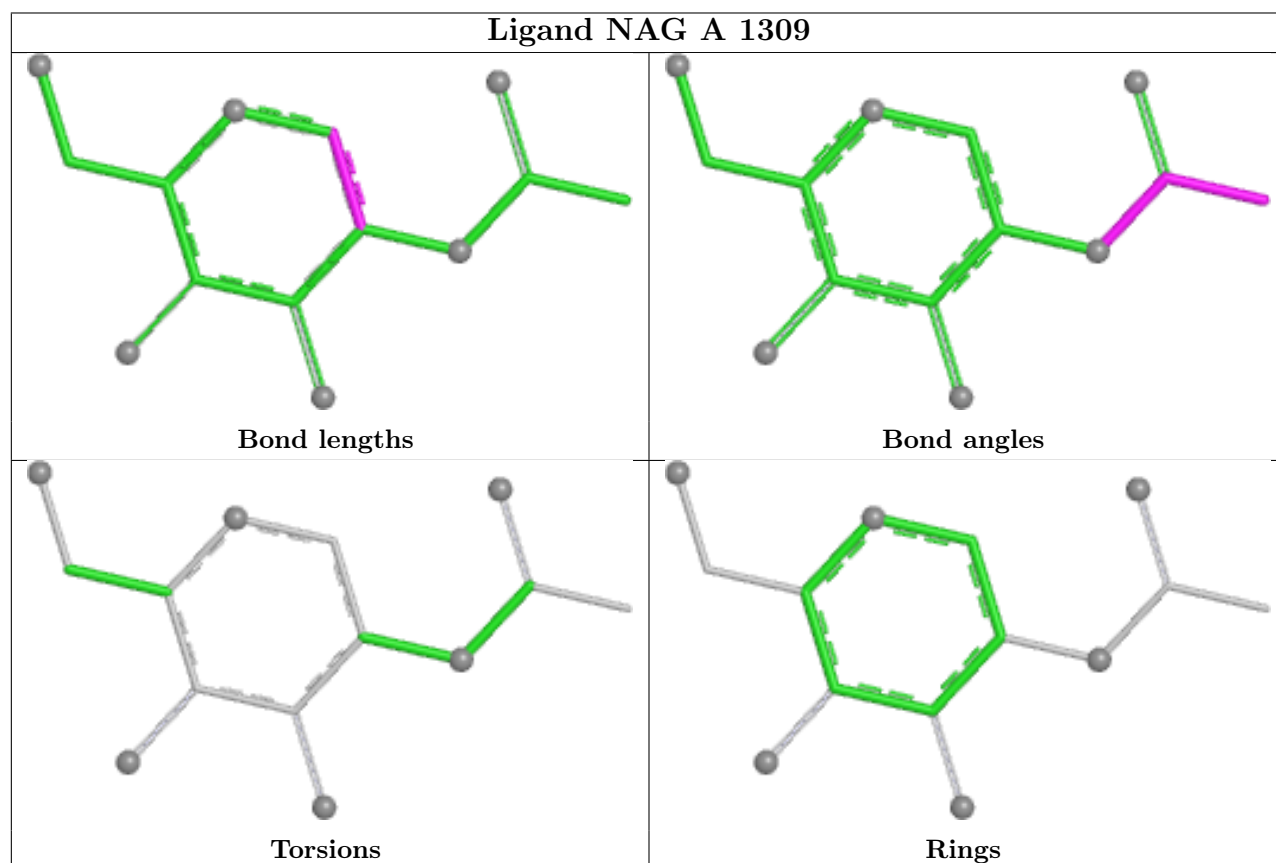
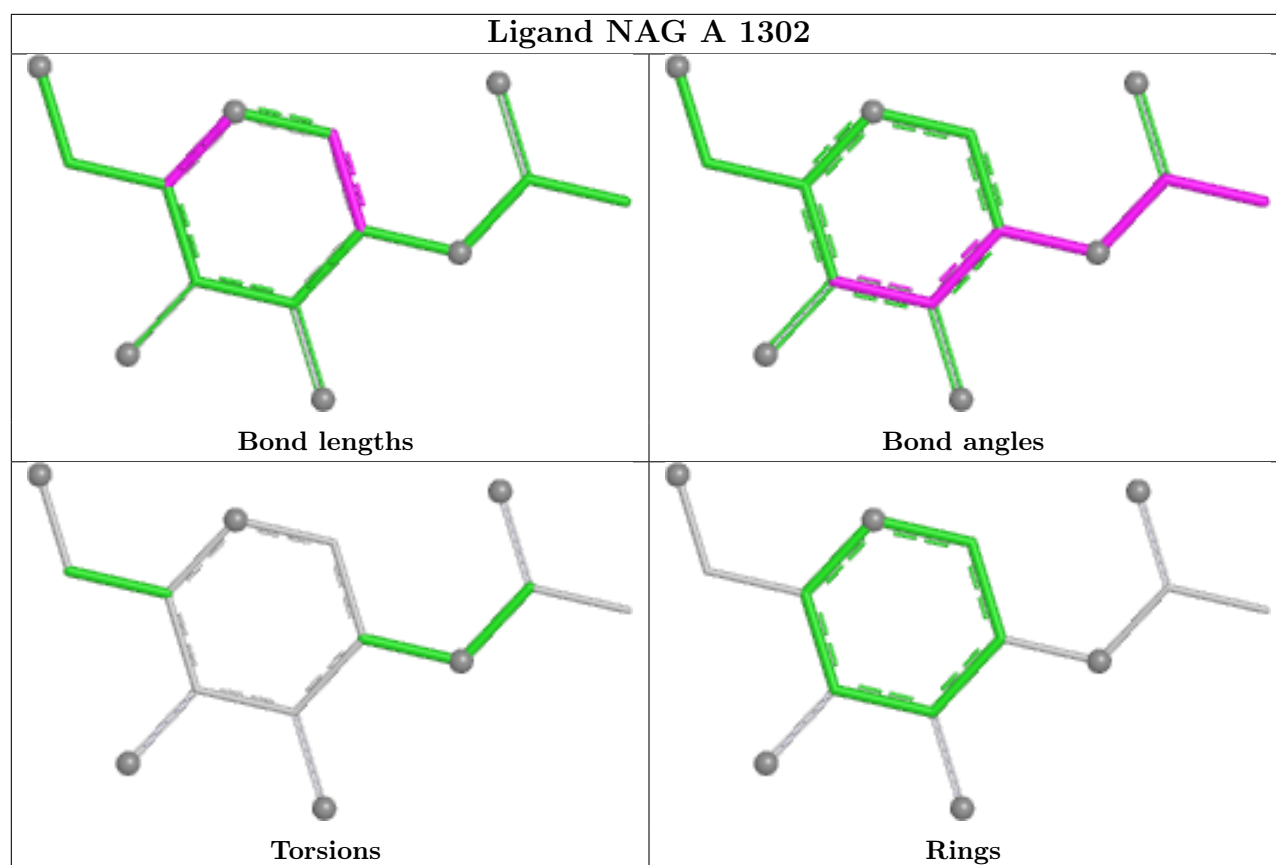


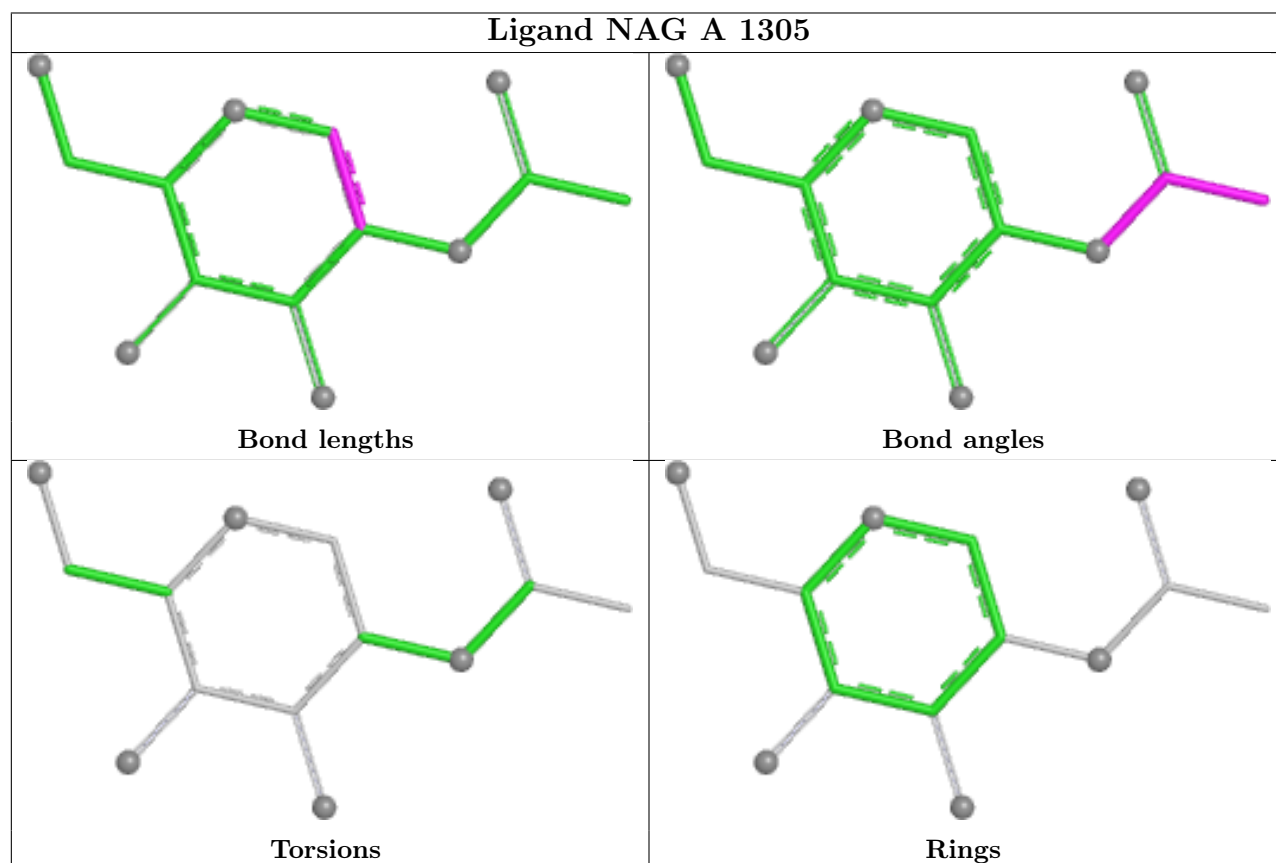
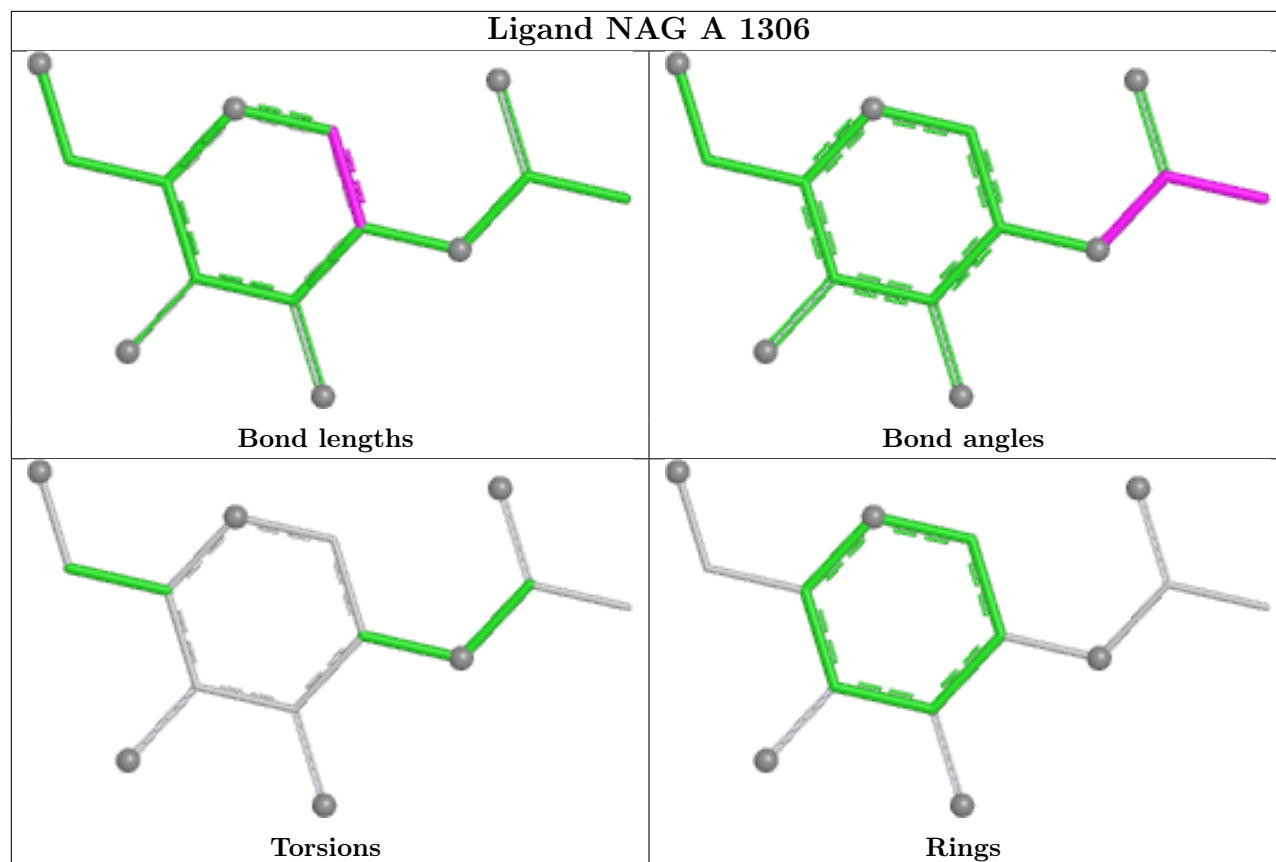
Ligand NAG B 1303



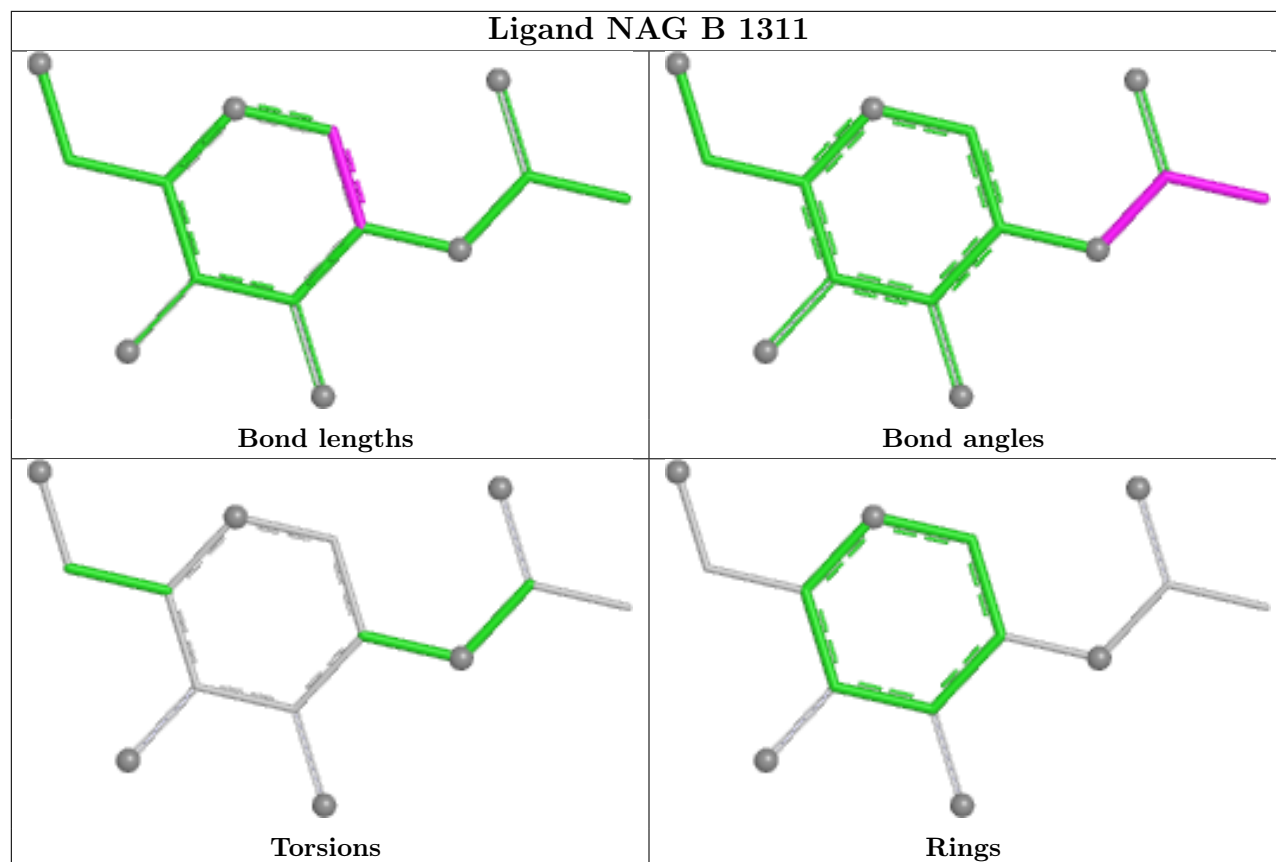
Ligand NAG C 1310



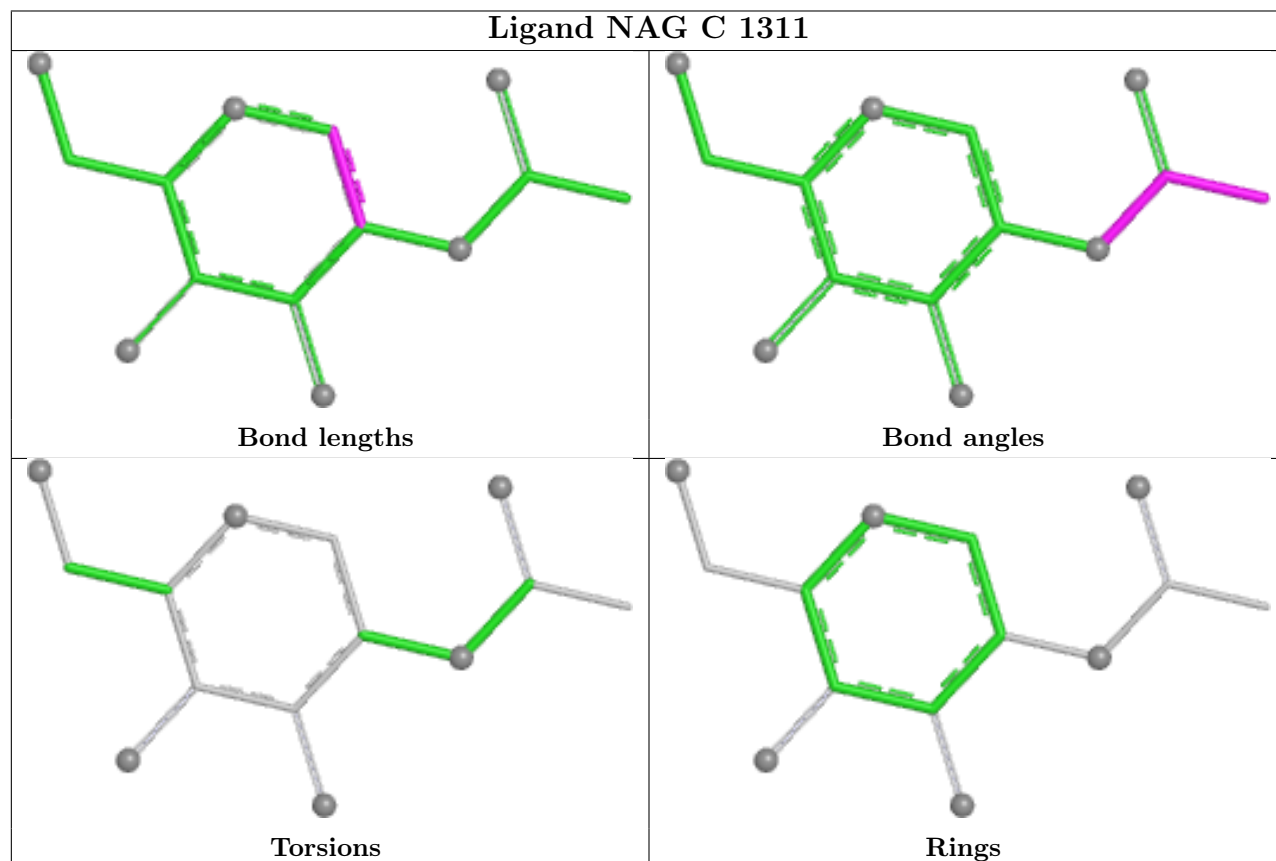


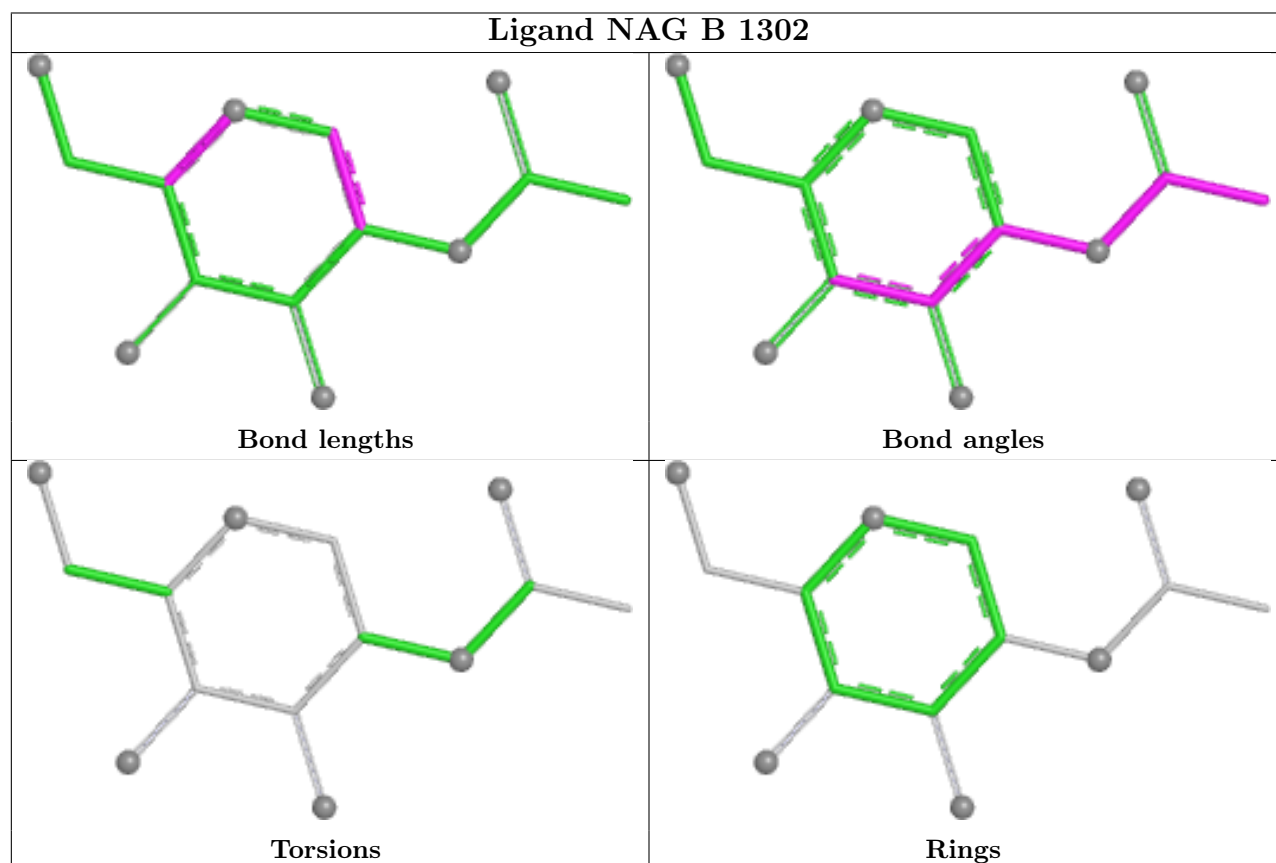
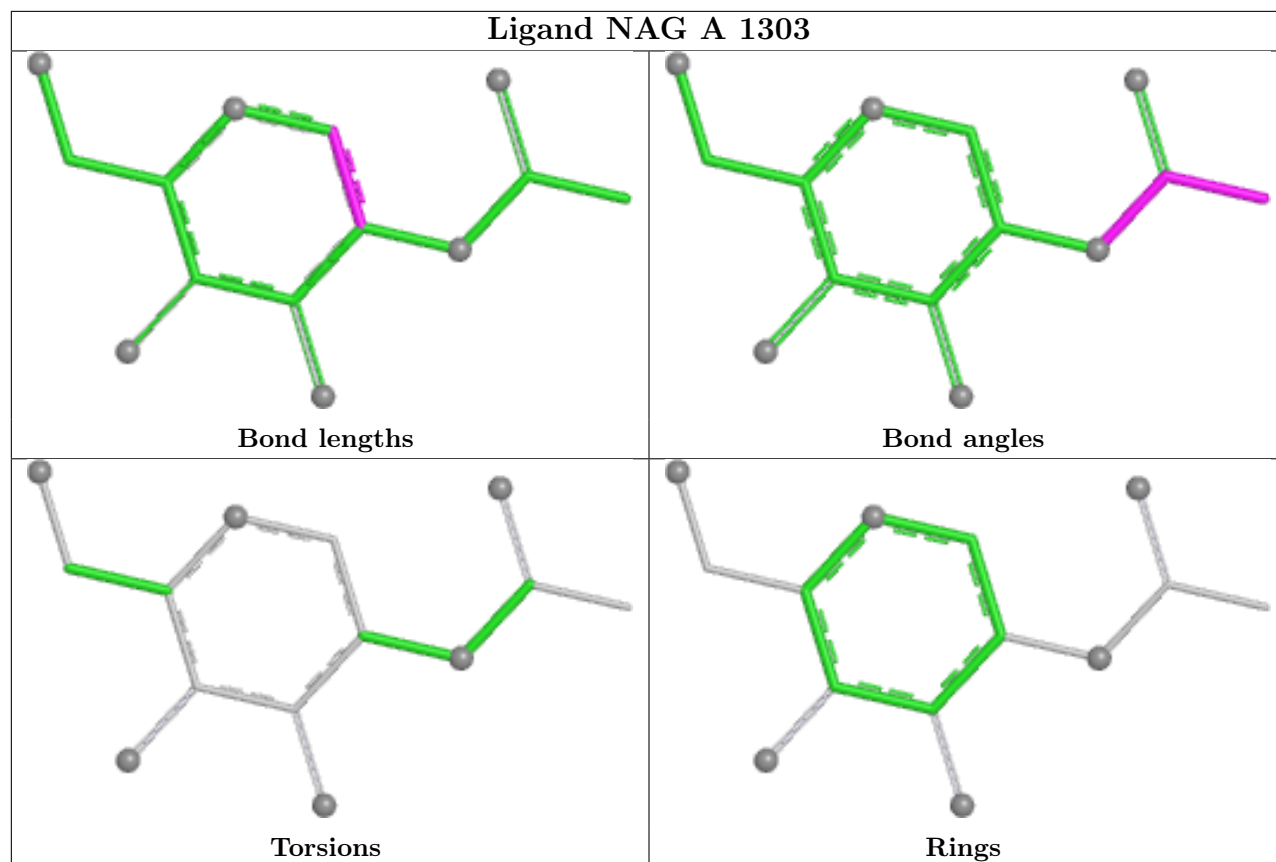


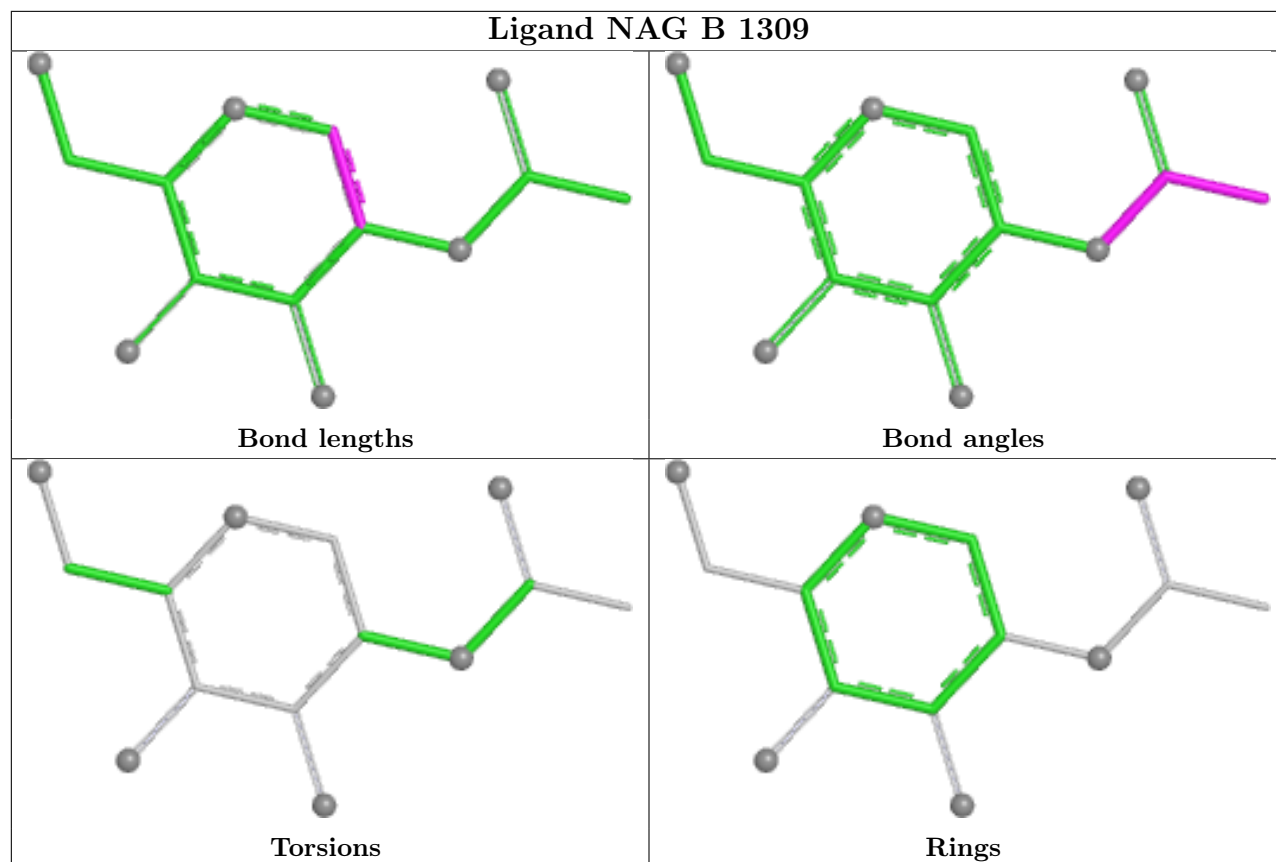
Ligand NAG B 1311



Ligand NAG C 1311







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.

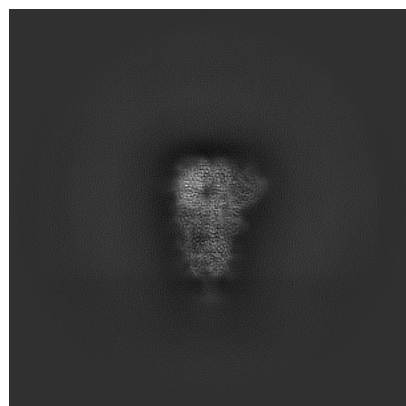
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41842. These allow visual inspection of the internal detail of the map and identification of artifacts.

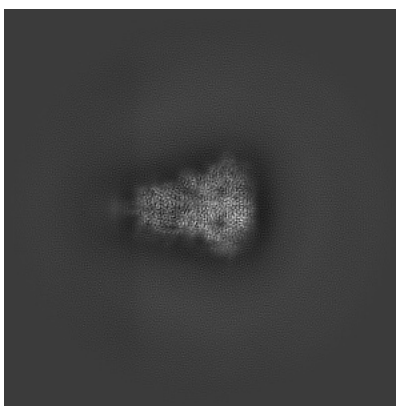
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

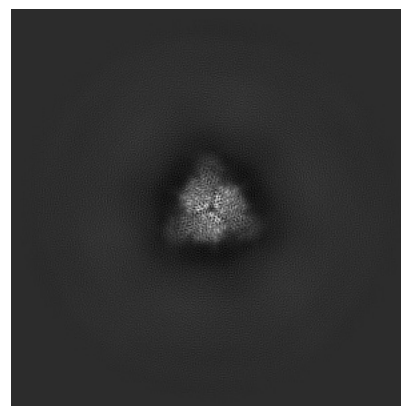
6.1.1 Primary map



X

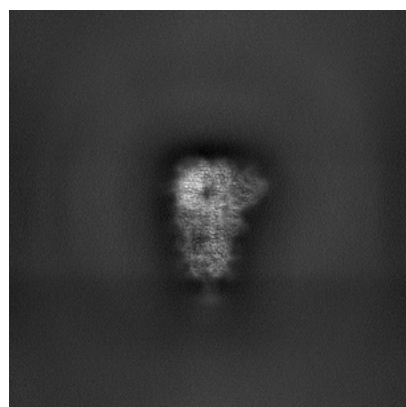


Y

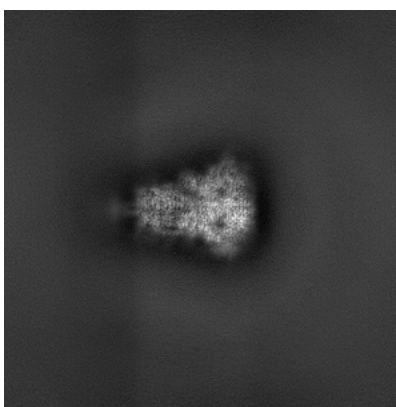


Z

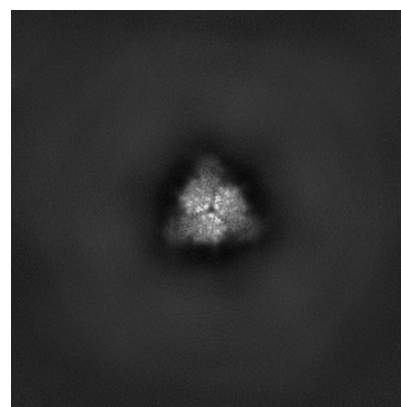
6.1.2 Raw map



X



Y

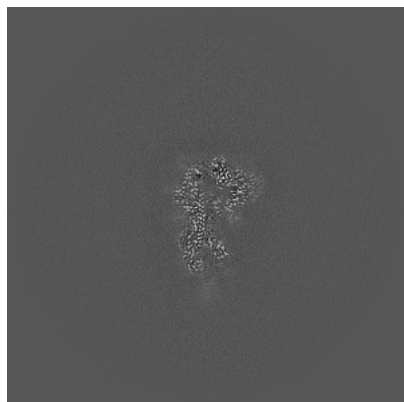


Z

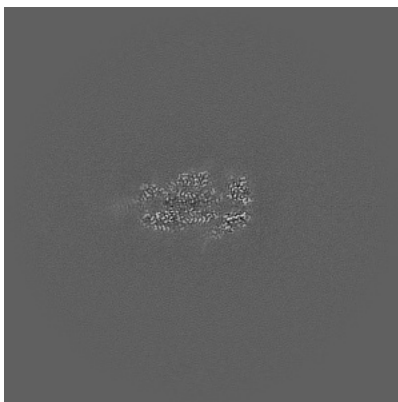
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

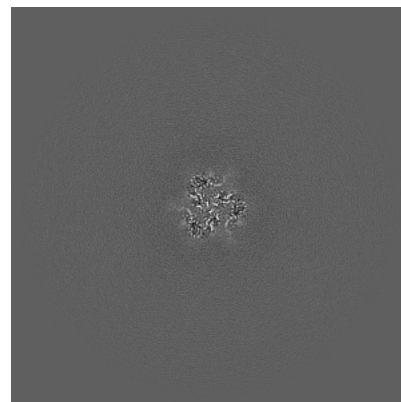
6.2.1 Primary map



X Index: 256

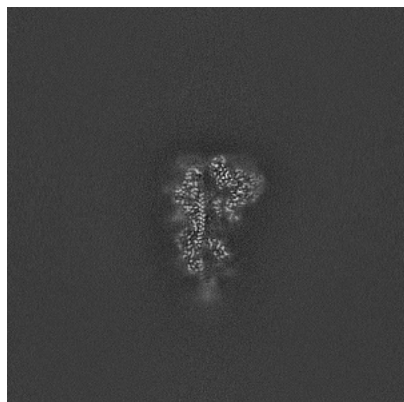


Y Index: 256

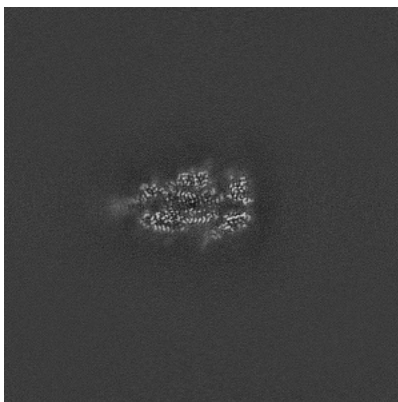


Z Index: 256

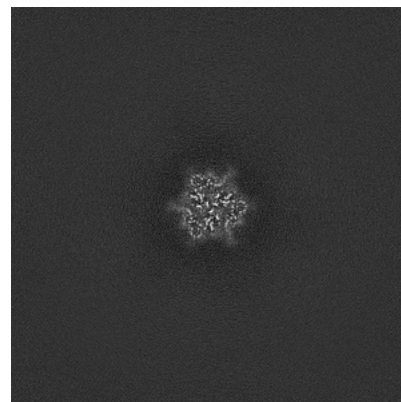
6.2.2 Raw map



X Index: 256



Y Index: 256

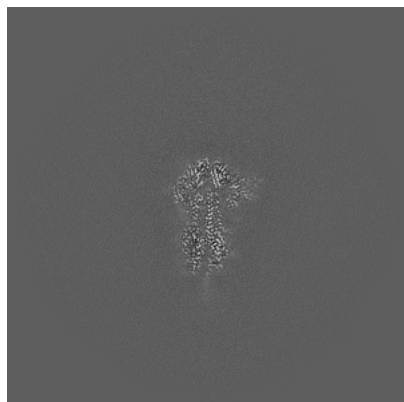


Z Index: 256

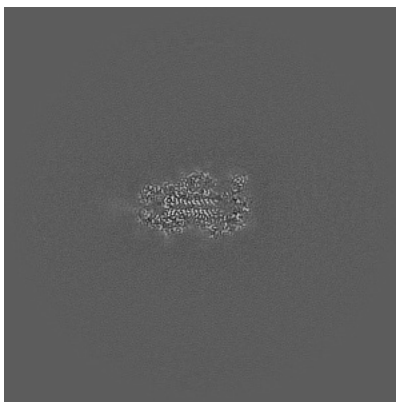
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

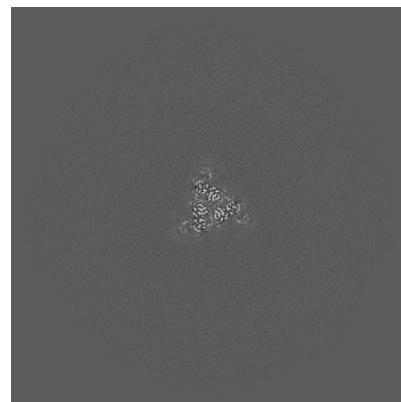
6.3.1 Primary map



X Index: 263

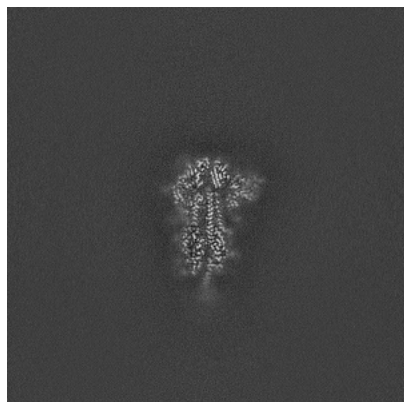


Y Index: 261

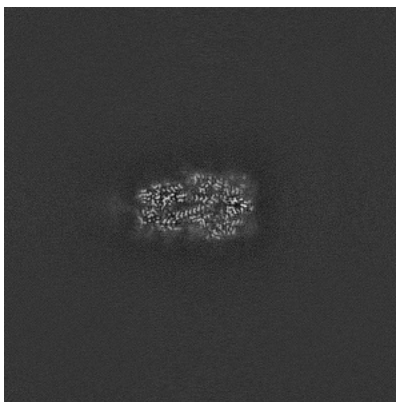


Z Index: 303

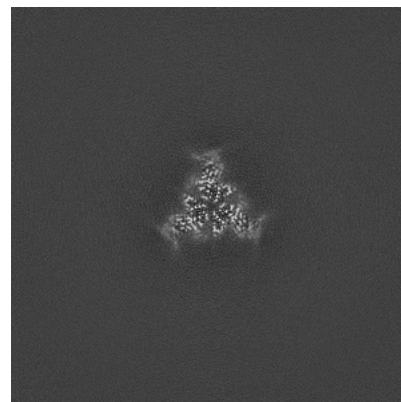
6.3.2 Raw map



X Index: 263



Y Index: 268

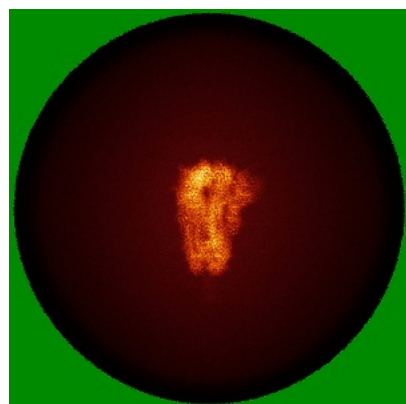


Z Index: 290

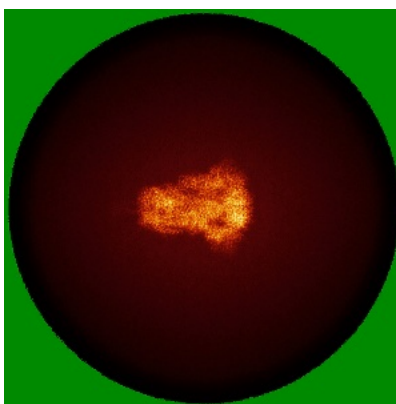
The images above show the largest variance slices of the map in three orthogonal directions.

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

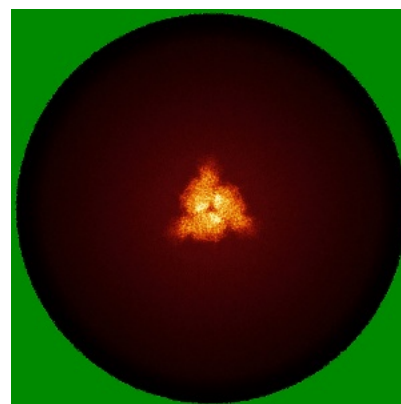
6.4.1 Primary map



X

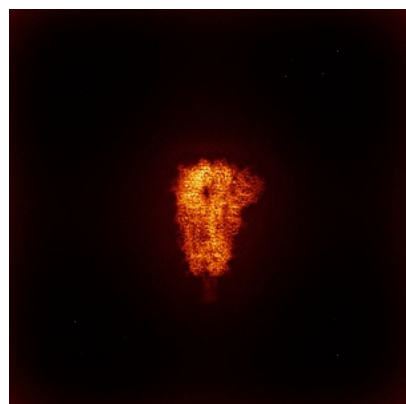


Y

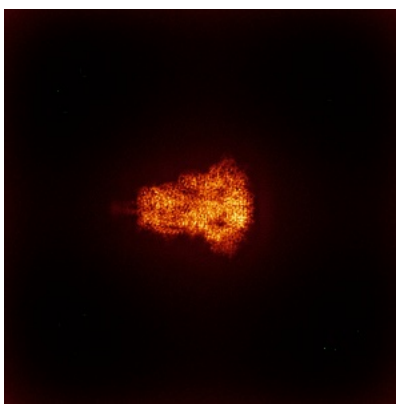


Z

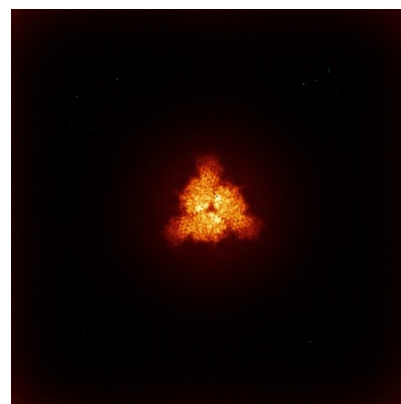
6.4.2 Raw map



X



Y

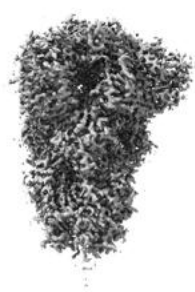


Z

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

6.5 Orthogonal surface views [i](#)

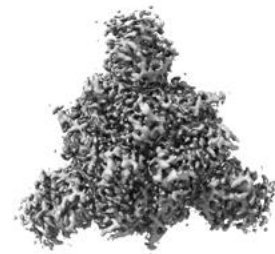
6.5.1 Primary map



X



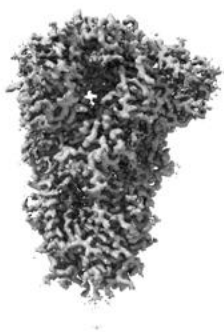
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

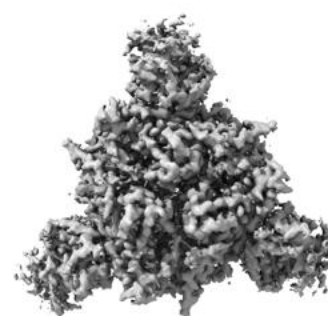
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

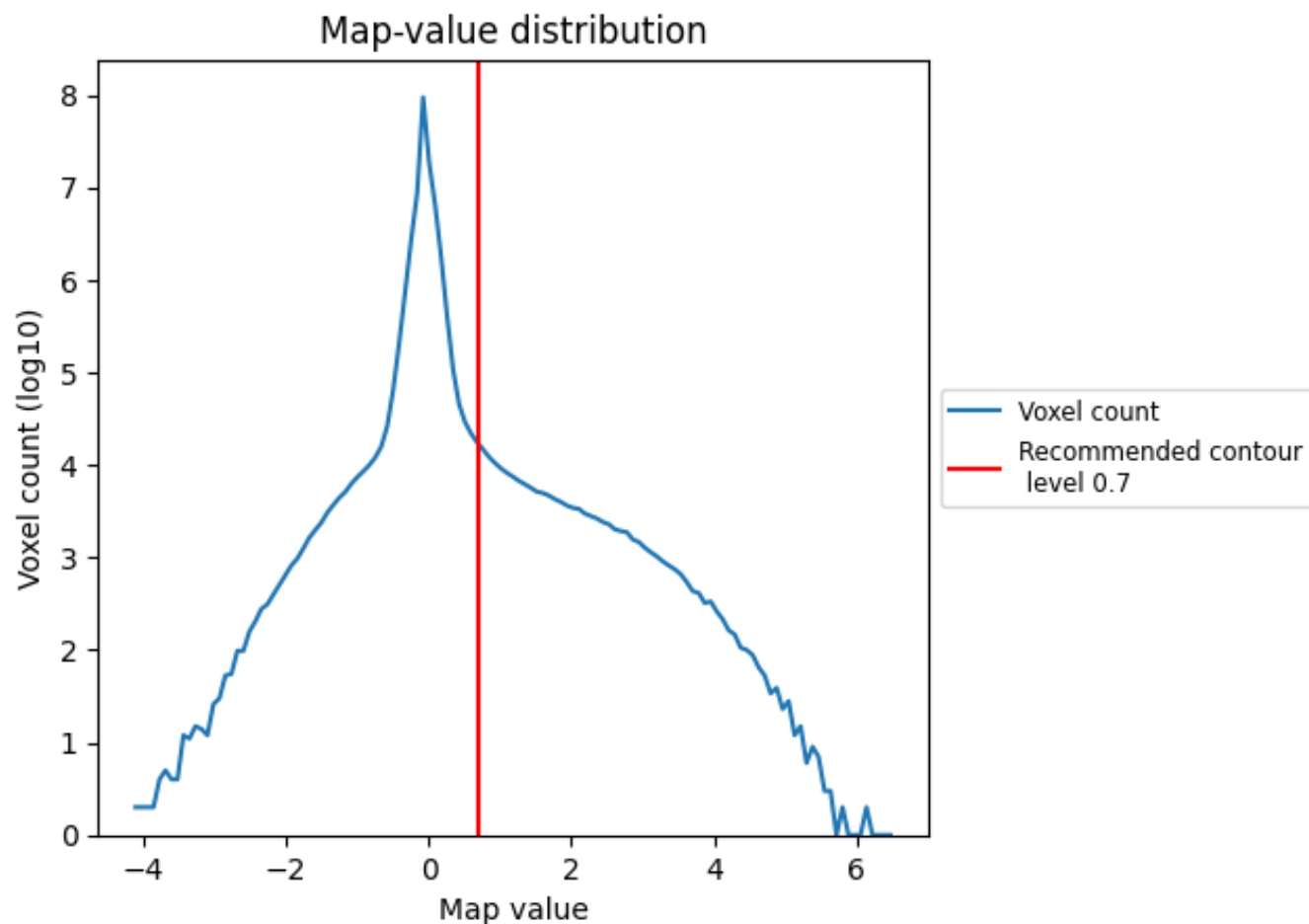
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

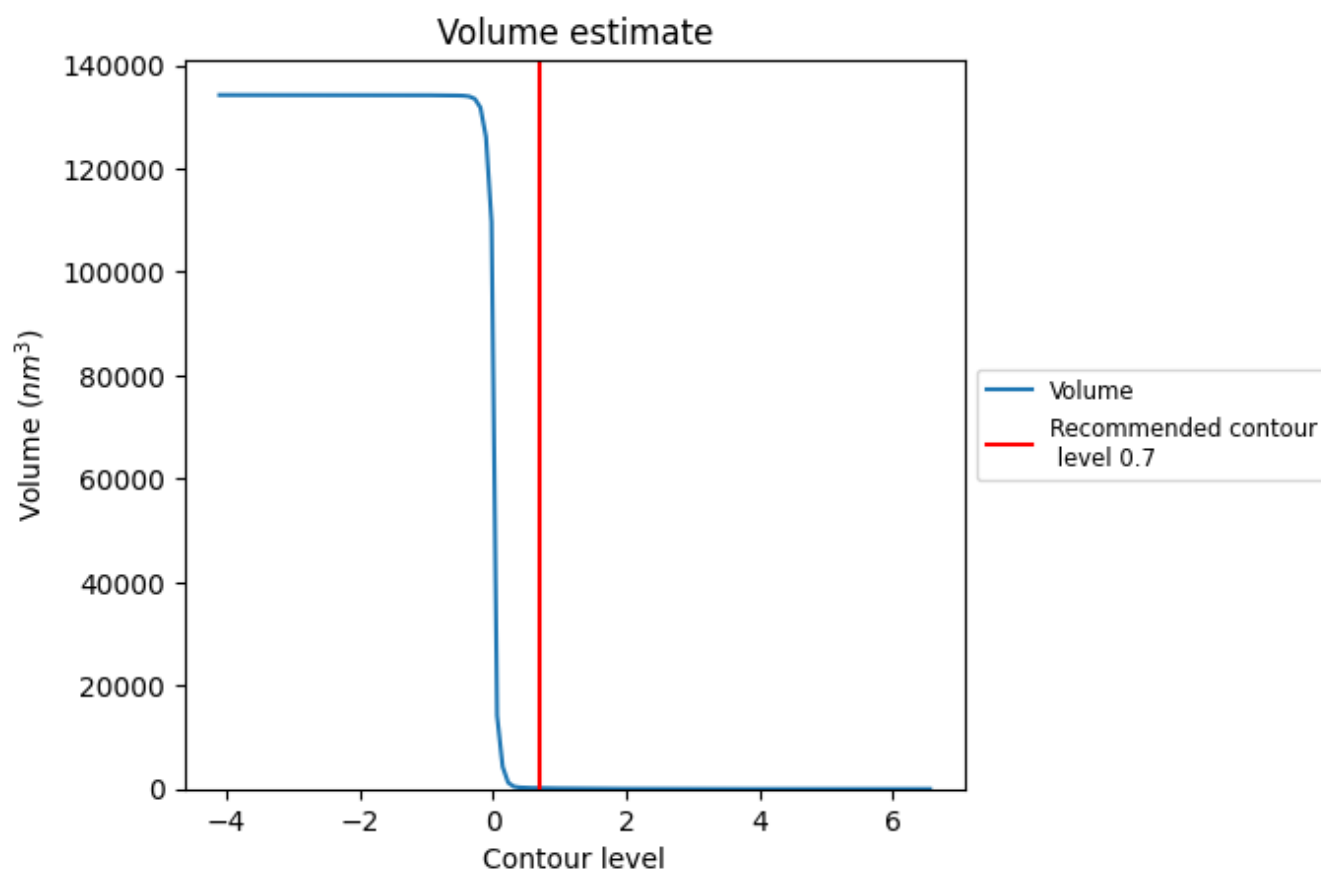
This section contains the results of statistical analysis of the map.

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.

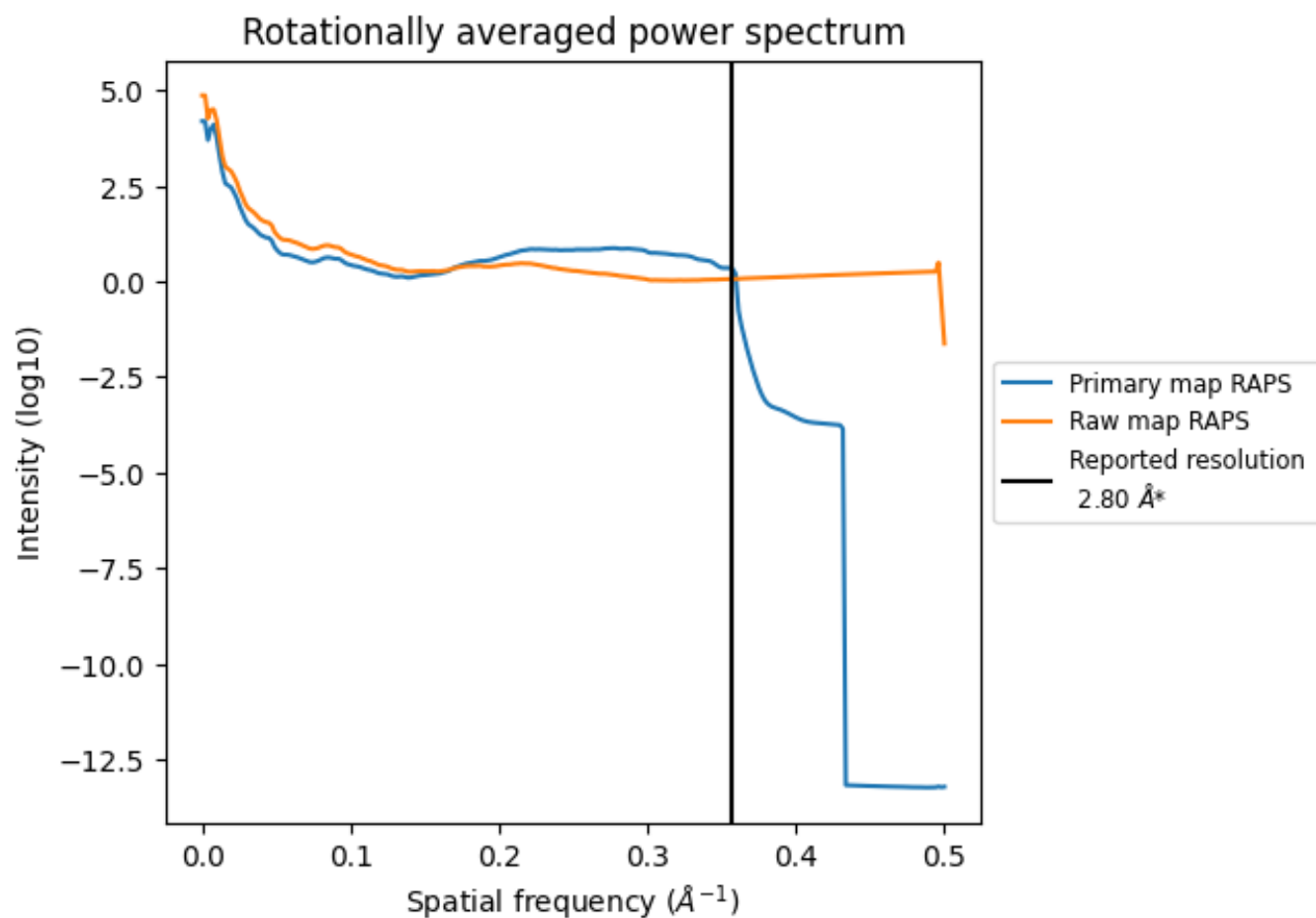
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm³; this corresponds to an approximate mass of 145 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

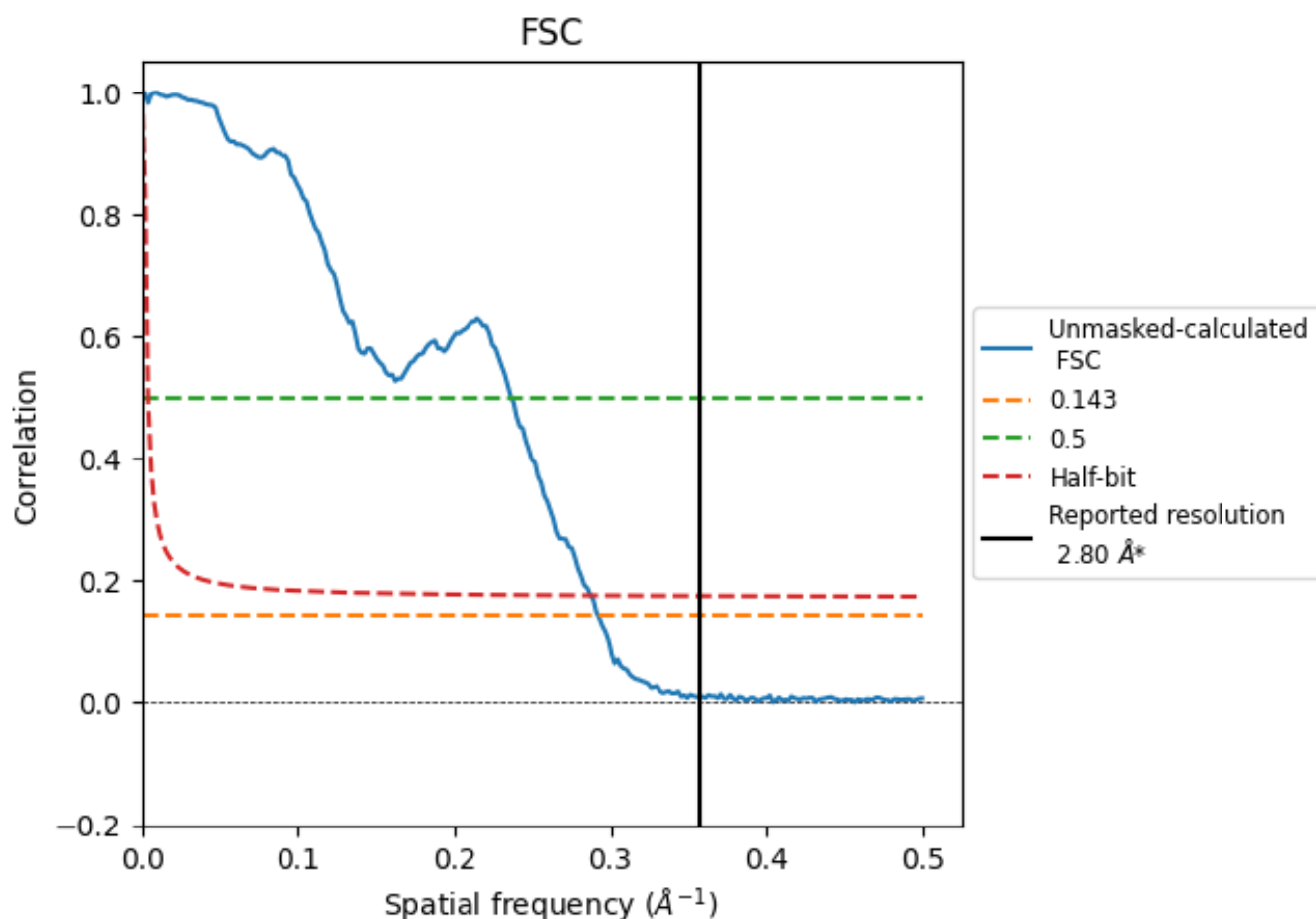


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

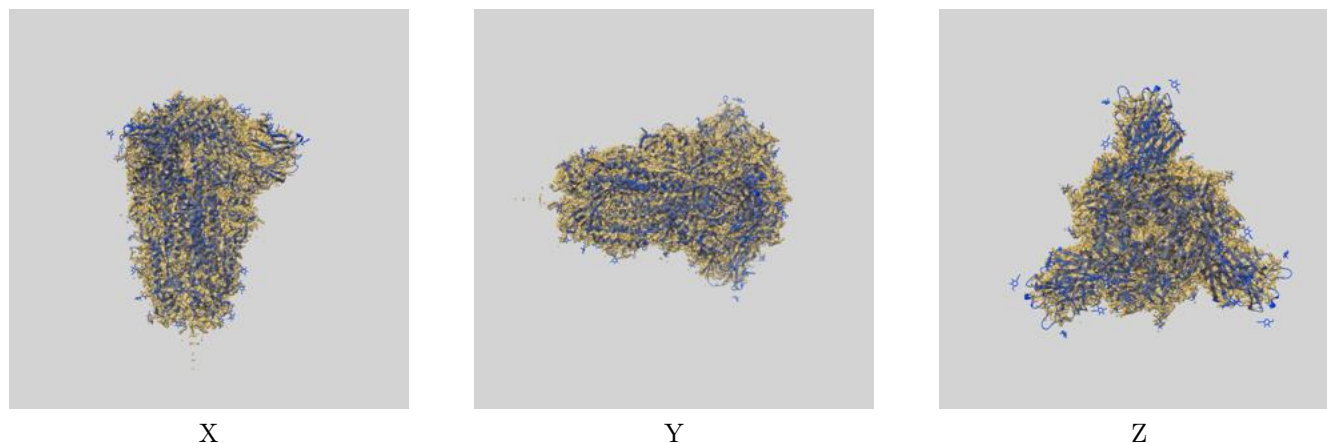
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.42	4.22	3.48

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

9 Map-model fit [i](#)

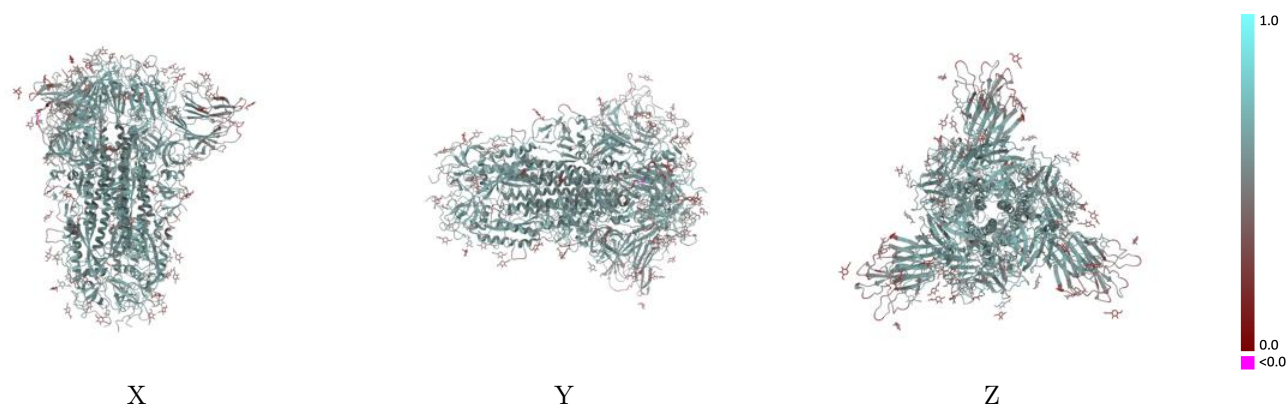
This section contains information regarding the fit between EMDB map EMD-41842 and PDB model 8U29. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



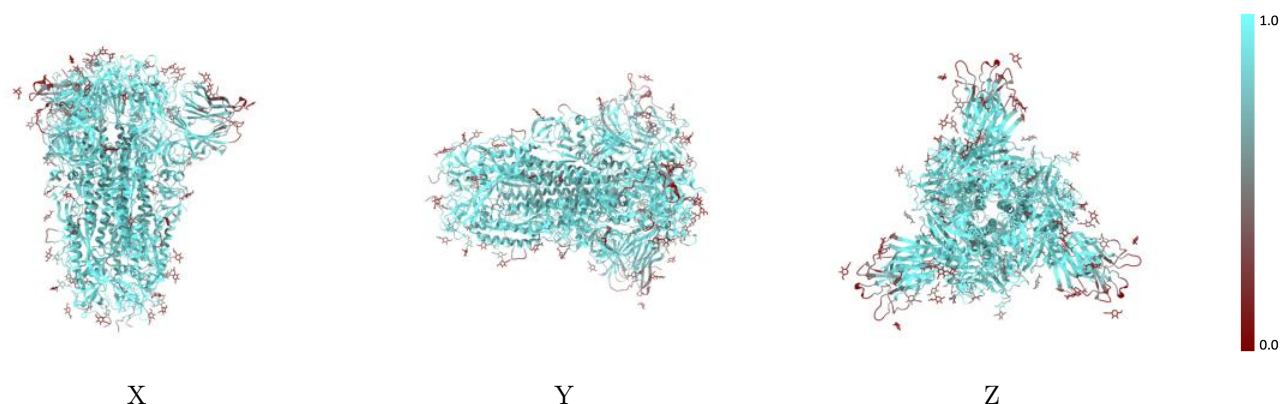
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



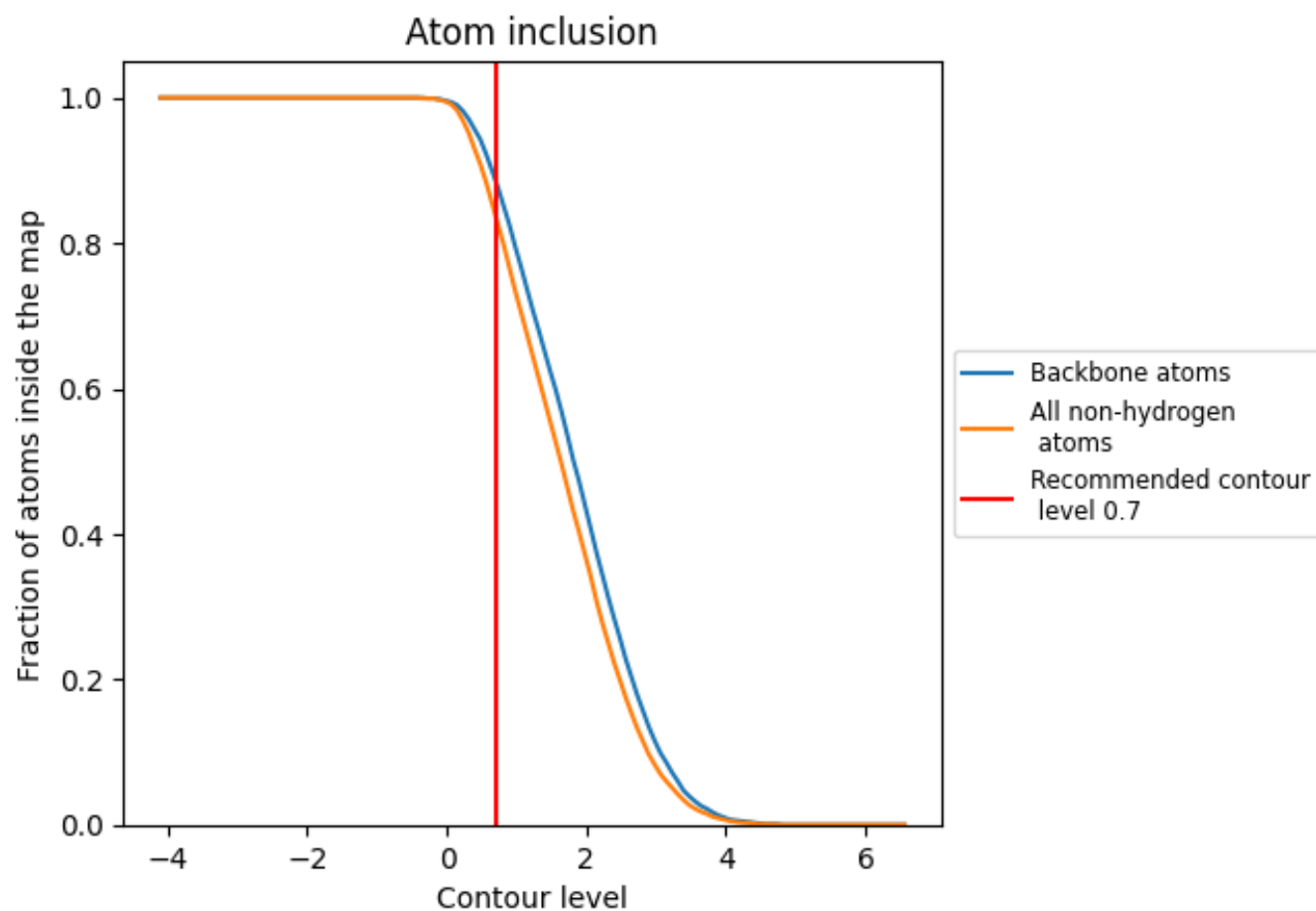
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.5640
A	 0.8610	 0.5730
B	 0.8620	 0.5720
C	 0.8610	 0.5720
D	 0.1070	 0.2550
E	 0.4290	 0.4390
F	 0.0360	 0.3160
G	 0.1200	 0.2800
H	 0.4720	 0.4040
I	 0.5360	 0.4050
J	 0.3570	 0.3180
K	 0.3210	 0.3010
L	 0.3930	 0.3660
M	 0.2500	 0.3620
N	 0.1070	 0.2770
O	 0.4290	 0.4470
P	 0.0360	 0.3240
Q	 0.1200	 0.2850
R	 0.4720	 0.4130
S	 0.5360	 0.4050
T	 0.3570	 0.3440
U	 0.2860	 0.2980
V	 0.3570	 0.3760
W	 0.2140	 0.3570
X	 0.1430	 0.2720
Y	 0.4290	 0.4670
Z	 0.0360	 0.3200
a	 0.1200	 0.2880
b	 0.4720	 0.4170
c	 0.5710	 0.4100
d	 0.3210	 0.3350
e	 0.2860	 0.2820
f	 0.3210	 0.3730
g	 0.2860	 0.3710

