



Full wwPDB EM Validation Report ⓘ

Oct 26, 2025 – 04:28 AM JST

PDB ID : 9KR8 / pdb_00009kr8
EMDB ID : EMD-62522
Title : Overall structure of HKU5 S protein in closed conformation
Authors : Zhang, Y.Y.; Xia, L.Y.; Zhou, Q.
Deposited on : 2024-11-27
Resolution : 2.39 Å(reported)

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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:

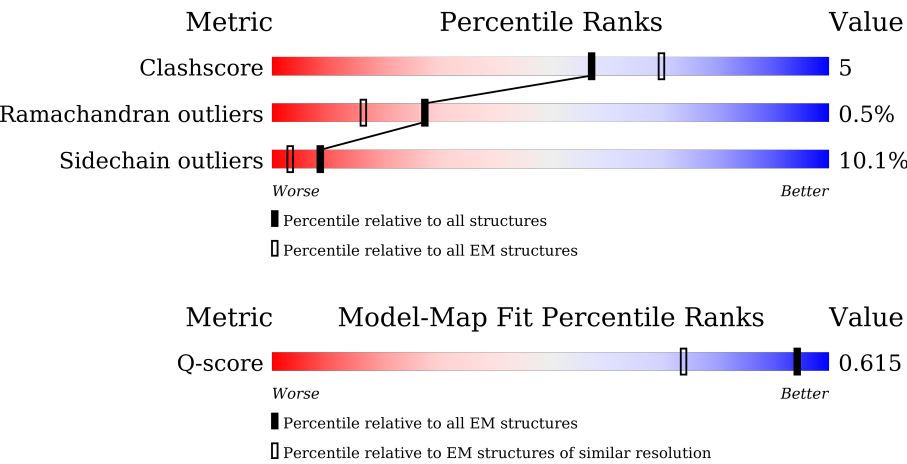
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.46

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.39 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.



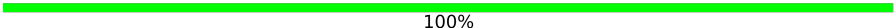

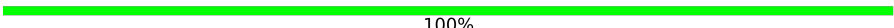








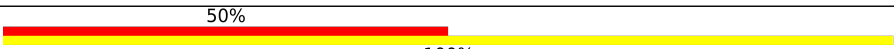
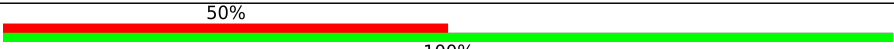





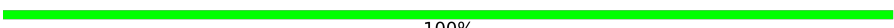



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	4884 (1.90 - 2.89)

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	1352	<div><div>9%</div><div><div></div><div>73%</div><div>12%</div><div>•</div><div>14%</div></div></div>
1	B	1352	<div><div>8%</div><div><div></div><div>72%</div><div>13%</div><div>•</div><div>14%</div></div></div>
1	C	1352	<div><div>9%</div><div><div></div><div>70%</div><div>14%</div><div>•</div><div>14%</div></div></div>
2	D	2	<div><div></div><div><div>50%</div><div>50%</div></div></div>
2	E	2	<div><div></div><div><div>50%</div><div>50%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 50% 100%
2	H	2	 100%
2	I	2	 50% 50%
2	J	2	 50% 100%
2	K	2	 50% 50%
2	L	2	 50% 50%
2	M	2	 50% 100%
2	N	2	 50% 50%
2	O	2	 50% 50%
2	P	2	 100%
2	Q	2	 50% 100%
2	R	2	 50% 100%
2	S	2	 50% 50%
2	T	2	 50% 50%
2	U	2	 50% 100%
2	V	2	 50% 50%
2	W	2	 50% 50%
2	X	2	 100%
2	Y	2	 50% 50%
2	Z	2	 50% 100%
2	a	2	 50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLM	A	3001	-	-	X	-
3	PLM	B	2002	-	-	X	-
3	PLM	C	2002	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 28356 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	1163	Total	C	N	O	S	0	0
			9036	5737	1490	1759	50		
1	B	1163	Total	C	N	O	S	0	0
			9036	5737	1490	1759	50		
1	C	1163	Total	C	N	O	S	0	0
			9036	5737	1490	1759	50		

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



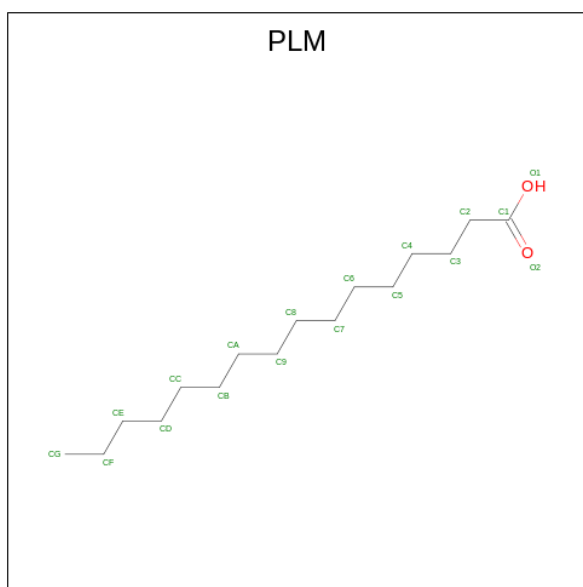
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16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

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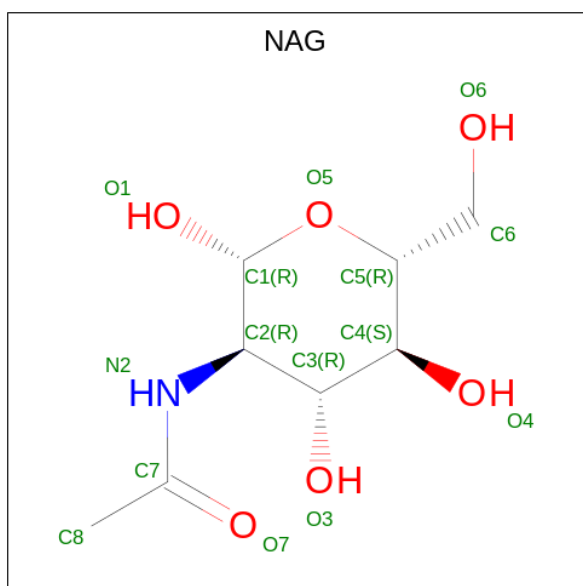
Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	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	a	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			18	16	2	
3	B	1	Total	C	O	0
			18	16	2	
3	C	1	Total	C	O	0
			18	16	2	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



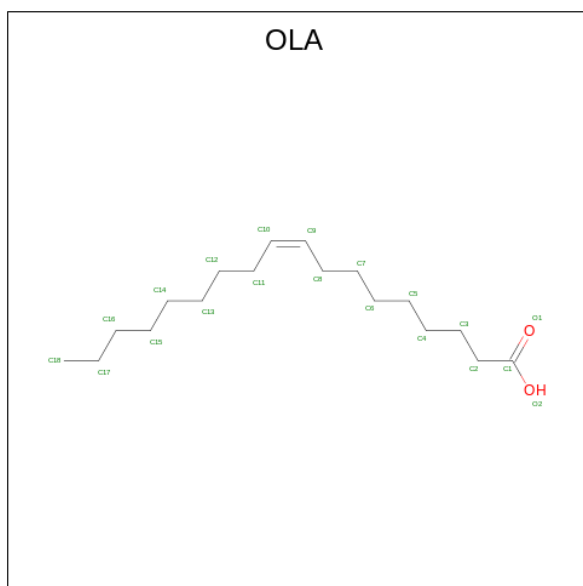
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4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

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

- Molecule 5 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$) (labeled as "Ligand of Interest" by depositor).

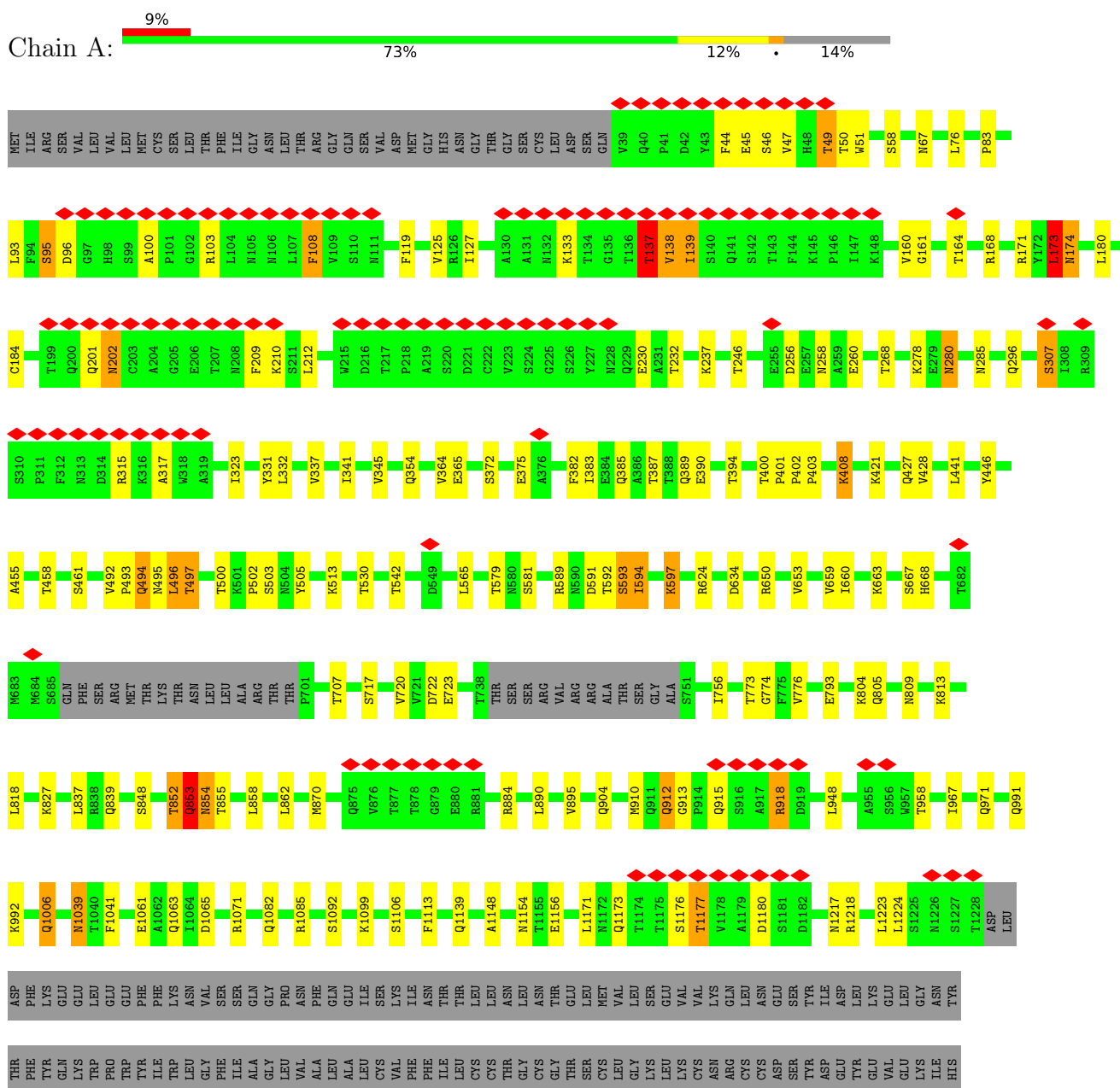


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			20	18	2	
5	B	1	Total	C	O	0
			20	18	2	
5	C	1	Total	C	O	0
			20	18	2	

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

Chain F:  100%



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

Chain G:  50%
100%



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

Chain H:  100%



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

Chain I:  50%
50% 50%



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

Chain J:  50%
100%



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

Chain K:  50% 50%



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

Chain L:  50% 50%



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

Chain M:  50% 100%



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

Chain N:  50% 50%



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

Chain O:  50% 50%



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

Chain P:  100%



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

Chain Q:  50% 100%



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



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



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



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



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



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



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

Chain X:  100%



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

Chain Y:  50%
 50%



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

Chain Z:  50%
 100%



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

Chain a:  50%
 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	801468	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.394	Depositor
Minimum map value	-4.198	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.168	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	347.84, 347.84, 347.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.36	0/9255	0.66	10/12610 (0.1%)
1	B	0.36	0/9255	0.65	10/12610 (0.1%)
1	C	0.35	0/9255	0.61	8/12610 (0.1%)
All	All	0.36	0/27765	0.64	28/37830 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	3
1	C	0	3
All	All	0	12

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	THR	N-CA-C	9.19	122.65	108.96
1	A	497	THR	CA-C-N	8.75	136.97	122.54
1	A	497	THR	C-N-CA	8.75	136.97	122.54
1	B	494	GLN	N-CA-C	6.96	119.72	111.71
1	A	495	ASN	N-CA-C	6.90	121.99	113.50
1	C	853	GLN	CA-C-N	6.80	134.53	121.54
1	C	853	GLN	C-N-CA	6.80	134.53	121.54
1	B	853	GLN	CA-C-N	6.63	134.21	121.54
1	B	853	GLN	C-N-CA	6.63	134.21	121.54
1	A	853	GLN	CA-C-N	6.61	134.16	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	GLN	C-N-CA	6.61	134.16	121.54
1	B	492	VAL	CA-C-N	5.97	125.93	119.78
1	B	492	VAL	C-N-CA	5.97	125.93	119.78
1	C	119	PHE	CA-C-N	5.89	132.79	121.54
1	C	119	PHE	C-N-CA	5.89	132.79	121.54
1	B	119	PHE	CA-C-N	5.86	132.74	121.54
1	B	119	PHE	C-N-CA	5.86	132.74	121.54
1	B	173	LEU	CA-C-N	5.71	132.45	121.54
1	B	173	LEU	C-N-CA	5.71	132.45	121.54
1	A	119	PHE	CA-C-N	5.60	132.24	121.54
1	A	119	PHE	C-N-CA	5.60	132.24	121.54
1	A	173	LEU	CA-C-N	5.59	132.21	121.54
1	A	173	LEU	C-N-CA	5.59	132.21	121.54
1	C	494	GLN	N-CA-C	5.52	122.57	110.80
1	C	173	LEU	CA-C-N	5.51	132.07	121.54
1	C	173	LEU	C-N-CA	5.51	132.07	121.54
1	C	495	ASN	N-CA-C	5.34	119.48	112.92
1	B	383	ILE	N-CA-C	5.04	119.81	109.34

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	THR	Peptide
1	A	164	THR	Peptide
1	A	173	LEU	Peptide
1	A	201	GLN	Peptide
1	A	382	PHE	Mainchain
1	A	387	THR	Peptide
1	B	173	LEU	Peptide
1	B	201	GLN	Peptide
1	B	382	PHE	Peptide
1	C	201	GLN	Peptide
1	C	382	PHE	Peptide
1	C	387	THR	Peptide

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	9036	0	8676	78	0
1	B	9036	0	8676	93	0
1	C	9036	0	8676	93	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	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
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
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	1	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	a	28	0	25	0	0
3	A	18	0	31	15	0
3	B	18	0	31	23	0
3	C	18	0	31	16	0
4	A	154	0	143	5	0
4	B	154	0	143	3	0
4	C	154	0	143	1	0
5	A	20	0	33	1	0
5	B	20	0	33	1	0
5	C	20	0	33	1	0
All	All	28356	0	27249	255	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 5.

All (255) 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:A:494:GLN:NE2	4:A:3007:NAG:H82	1.43	1.28
1:C:403:PRO:HD3	3:C:2002:PLM:CB	1.68	1.21
1:B:403:PRO:HD3	3:B:2002:PLM:CB	1.73	1.19
1:B:403:PRO:HD3	3:B:2002:PLM:HB1	1.27	1.11
1:A:494:GLN:HE22	4:A:3007:NAG:C8	1.62	1.10
1:C:403:PRO:HD3	3:C:2002:PLM:HB2	1.17	1.09
1:C:403:PRO:CD	3:C:2002:PLM:HB2	1.85	1.06
1:A:494:GLN:HE22	4:A:3007:NAG:H82	0.86	1.01
1:C:455:ALA:O	3:C:2002:PLM:H51	1.71	0.91
1:A:401:PRO:O	3:A:3001:PLM:H92	1.70	0.91
1:C:403:PRO:HD3	3:C:2002:PLM:HB1	1.55	0.87
1:A:403:PRO:HA	3:A:3001:PLM:H52	1.56	0.86
1:A:505:TYR:HA	3:A:3001:PLM:H62	1.57	0.85
1:B:400:THR:O	3:B:2002:PLM:CF	2.23	0.85
1:B:403:PRO:HB3	3:B:2002:PLM:H72	1.56	0.85
1:B:402:PRO:HA	3:B:2002:PLM:HB2	1.61	0.83
1:C:506:ALA:H	3:C:2002:PLM:H61	1.44	0.82
1:A:400:THR:O	3:A:3001:PLM:HE1	1.80	0.82
1:B:403:PRO:CD	3:B:2002:PLM:CB	2.56	0.82
1:B:403:PRO:CD	3:B:2002:PLM:HB1	2.08	0.82
1:B:403:PRO:HD3	3:B:2002:PLM:HB2	1.62	0.81
1:B:400:THR:O	3:B:2002:PLM:HF1	1.83	0.79
1:C:455:ALA:O	3:C:2002:PLM:C5	2.31	0.78
1:C:505:TYR:HA	3:C:2002:PLM:H72	1.66	0.78
1:B:494:GLN:HE22	4:B:2008:NAG:H82	1.51	0.74
1:A:493:PRO:HG2	1:A:496:LEU:HD22	1.70	0.74
1:B:496:LEU:O	1:B:497:THR:OG1	2.06	0.73
1:C:494:GLN:CD	1:C:494:GLN:H	1.94	0.72
1:B:403:PRO:CD	3:B:2002:PLM:HB2	2.20	0.71
1:B:285:ASN:HD21	1:B:341:ILE:H	1.37	0.70
1:A:285:ASN:HD21	1:A:341:ILE:H	1.39	0.69
1:A:402:PRO:HA	3:A:3001:PLM:HD2	1.73	0.69
1:A:403:PRO:HD3	3:A:3001:PLM:H91	1.75	0.69
1:C:496:LEU:O	1:C:497:THR:OG1	2.08	0.68
1:A:912:GLN:HE21	1:B:650:ARG:HD3	1.61	0.66
1:B:505:TYR:HB3	3:B:2002:PLM:H31	1.80	0.63
1:A:137:THR:HG22	1:A:317:ALA:HA	1.81	0.63
1:A:910:MET:SD	1:B:650:ARG:NH1	2.72	0.62
1:C:104:LEU:HD13	1:C:309:ARG:HD3	1.81	0.62
1:B:1006:GLN:HE21	1:B:1006:GLN:H	1.48	0.61
1:C:455:ALA:HB3	3:C:2002:PLM:H71	1.83	0.61
1:C:1006:GLN:H	1:C:1006:GLN:HE21	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:PRO:CB	3:B:2002:PLM:H72	2.29	0.61
1:C:400:THR:O	3:C:2002:PLM:CF	2.48	0.61
1:B:400:THR:O	3:B:2002:PLM:HG1	2.01	0.61
1:C:151:TYR:O	1:C:306:ARG:NH1	2.34	0.61
1:B:1155:THR:H	1:B:1159:GLN:HE21	1.49	0.60
1:C:496:LEU:HD12	1:C:496:LEU:N	2.16	0.60
1:A:593:SER:O	1:A:597:LYS:NZ	2.35	0.59
1:A:455:ALA:O	3:A:3001:PLM:H41	2.02	0.59
1:B:107:LEU:HD23	1:B:307:SER:HB2	1.84	0.59
1:A:258:ASN:ND2	1:A:280:ASN:OD1	2.36	0.59
1:B:400:THR:O	3:B:2002:PLM:CG	2.50	0.58
1:C:400:THR:HB	3:C:2002:PLM:HF2	1.85	0.58
1:A:168:ARG:NH2	1:A:209:PHE:O	2.36	0.58
1:A:809:ASN:HD21	1:A:1071:ARG:HH12	1.52	0.58
1:A:1217:ASN:HD22	1:A:1218:ARG:HG3	1.69	0.58
1:B:127:ILE:HB	1:B:260:GLU:HB3	1.85	0.58
1:B:137:THR:OG1	1:B:138:VAL:N	2.37	0.58
1:C:402:PRO:HA	3:C:2002:PLM:HD2	1.85	0.58
1:B:125:VAL:HG22	1:B:323:ILE:HG12	1.86	0.57
1:A:49:THR:OG1	1:A:50:THR:N	2.36	0.57
1:A:127:ILE:HB	1:A:260:GLU:HB3	1.86	0.57
1:B:354:GLN:NE2	1:B:372:SER:OG	2.38	0.57
1:C:354:GLN:NE2	1:C:372:SER:OG	2.38	0.57
1:A:337:VAL:HG11	4:A:3002:NAG:H82	1.85	0.57
1:A:100:ALA:HB3	1:A:103:ARG:HB2	1.85	0.57
1:B:403:PRO:HA	3:B:2002:PLM:H52	1.86	0.56
1:A:83:PRO:O	1:A:331:TYR:OH	2.22	0.56
1:B:138:VAL:O	1:B:141:GLN:NE2	2.38	0.56
1:B:202:ASN:N	1:B:202:ASN:OD1	2.38	0.56
1:B:1099:LYS:NZ	1:B:1113:PHE:O	2.37	0.56
1:C:400:THR:O	3:C:2002:PLM:HF2	2.05	0.56
1:C:502:PRO:HG3	3:C:2002:PLM:HA2	1.86	0.56
1:A:1006:GLN:H	1:A:1006:GLN:HE21	1.54	0.56
1:B:438:PRO:HB3	5:C:2001:OLA:H52	1.88	0.56
1:A:137:THR:OG1	1:A:138:VAL:N	2.28	0.55
1:A:458:THR:O	1:A:461:SER:HB3	2.06	0.55
1:A:1099:LYS:NZ	1:A:1113:PHE:O	2.39	0.55
1:B:460:MET:SD	3:B:2002:PLM:O1	2.65	0.55
1:B:910:MET:SD	1:C:650:ARG:NH1	2.77	0.55
1:A:496:LEU:N	1:A:496:LEU:HD13	2.21	0.55
1:B:196:HIS:HB3	1:B:241:ASP:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:PRO:HG2	1:C:496:LEU:HD13	1.87	0.55
1:C:365:GLU:OE1	1:C:663:LYS:NZ	2.39	0.55
1:C:168:ARG:NH2	1:C:209:PHE:O	2.40	0.54
1:C:100:ALA:HB3	1:C:103:ARG:HB2	1.90	0.54
1:C:337:VAL:HG11	4:C:2003:NAG:H82	1.90	0.54
1:A:918:ARG:HH11	1:A:918:ARG:HA	1.72	0.53
1:C:256:ASP:OD1	1:C:256:ASP:N	2.39	0.53
1:C:421:LYS:HD2	2:V:1:NAG:H61	1.90	0.53
1:A:400:THR:HB	3:A:3001:PLM:HE2	1.90	0.53
1:B:256:ASP:OD2	1:B:258:ASN:ND2	2.40	0.53
1:C:42:ASP:OD1	1:C:42:ASP:N	2.38	0.52
1:C:96:ASP:HB2	1:C:318:TRP:HE1	1.74	0.52
1:C:107:LEU:HD21	1:C:215:TRP:HE3	1.75	0.52
1:B:505:TYR:HA	3:B:2002:PLM:H62	1.91	0.52
1:C:496:LEU:C	1:C:497:THR:HG1	2.13	0.52
1:A:365:GLU:OE1	1:A:663:LYS:NZ	2.43	0.52
1:A:1039:ASN:HD22	1:A:1041:PHE:H	1.58	0.52
1:A:502:PRO:HG3	3:A:3001:PLM:H82	1.92	0.52
1:A:385:GLN:NE2	1:A:589:ARG:O	2.37	0.51
1:B:910:MET:HE1	1:C:653:VAL:HG21	1.93	0.51
1:A:403:PRO:CD	3:A:3001:PLM:H91	2.39	0.51
1:B:593:SER:O	1:B:597:LYS:NZ	2.41	0.51
1:C:681:THR:HA	1:C:684:MET:HE2	1.93	0.51
1:C:1181:SER:O	1:C:1218:ARG:NE	2.43	0.51
1:A:496:LEU:N	1:A:496:LEU:CD1	2.73	0.51
1:B:96:ASP:HB2	1:B:318:TRP:HE1	1.75	0.51
1:B:99:SER:OG	1:B:315:ARG:NH2	2.43	0.51
1:B:137:THR:HB	1:B:318:TRP:H	1.75	0.51
1:A:793:GLU:O	1:A:1092:SER:OG	2.23	0.50
1:A:125:VAL:HG22	1:A:323:ILE:HG12	1.92	0.50
1:B:456:TYR:CD1	3:B:2002:PLM:H22	2.47	0.50
1:A:44:PHE:HE1	1:A:95:SER:HB3	1.76	0.50
1:A:650:ARG:NH1	1:C:910:MET:SD	2.75	0.50
1:C:912:GLN:OE1	1:C:913:GLY:N	2.41	0.50
1:A:494:GLN:NE2	4:A:3007:NAG:C8	2.36	0.50
1:B:312:PHE:HA	1:B:315:ARG:HH21	1.77	0.50
1:B:586:GLN:O	1:B:589:ARG:NH2	2.45	0.49
1:B:366:THR:HG23	1:B:662:ASP:HA	1.93	0.49
1:C:809:ASN:HD21	1:C:1071:ARG:HH12	1.61	0.49
1:B:183:GLY:O	1:B:186:THR:OG1	2.28	0.49
1:C:258:ASN:ND2	1:C:280:ASN:OD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:THR:HB	3:B:2002:PLM:HF2	1.95	0.49
1:C:112:TYR:HB2	1:C:305:PRO:HG3	1.94	0.49
1:C:403:PRO:N	3:C:2002:PLM:HB2	2.27	0.49
1:A:428:VAL:HG21	5:B:2001:OLA:H22	1.94	0.49
1:B:717:SER:OG	1:B:756:ILE:O	2.31	0.48
1:C:660:ILE:O	1:C:668:HIS:HA	2.12	0.48
1:B:104:LEU:HD22	1:B:309:ARG:HG2	1.96	0.48
1:C:751:SER:OG	1:C:752:ASP:N	2.46	0.48
5:A:3013:OLA:H22	1:C:428:VAL:HG21	1.95	0.48
1:A:1082:GLN:HE22	1:A:1085:ARG:HH11	1.62	0.48
1:C:84:LYS:HB2	1:C:87:ASP:HB2	1.96	0.48
1:A:95:SER:O	1:A:307:SER:OG	2.29	0.48
1:A:707:THR:HA	1:C:903:MET:HG3	1.95	0.47
1:B:161:GLY:HA3	1:B:173:LEU:HD21	1.95	0.47
1:B:337:VAL:HG11	4:B:2003:NAG:H82	1.96	0.47
1:B:867:ASN:OD1	1:B:869:THR:OG1	2.32	0.47
1:B:898:ALA:HA	1:B:919:ASP:HB2	1.95	0.47
1:B:1087:GLU:OE1	1:B:1091:ARG:NH1	2.48	0.47
1:B:912:GLN:OE1	1:B:913:GLY:N	2.44	0.47
1:B:42:ASP:O	1:B:46:SER:OG	2.32	0.47
1:C:425:LEU:HD22	1:C:497:THR:HG23	1.96	0.47
1:A:400:THR:HG22	3:A:3001:PLM:HB1	1.96	0.47
1:A:717:SER:OG	1:A:756:ILE:O	2.32	0.47
1:B:402:PRO:HA	3:B:2002:PLM:HD2	1.97	0.47
1:B:506:ALA:O	3:B:2002:PLM:H51	2.15	0.47
1:C:117:GLU:HG3	1:C:301:TYR:CZ	2.49	0.47
1:C:94:PHE:HD2	1:C:150:ILE:HG21	1.79	0.47
1:A:722:ASP:OD1	1:A:722:ASP:N	2.45	0.47
1:C:260:GLU:OE1	1:C:283:ARG:NH1	2.47	0.47
1:A:400:THR:OG1	1:A:500:THR:OG1	2.30	0.47
1:A:502:PRO:CG	3:A:3001:PLM:H82	2.45	0.47
1:C:313:ASN:OD1	1:C:313:ASN:N	2.42	0.47
1:C:796:ILE:H	1:C:839:GLN:HE22	1.61	0.47
1:B:921:ILE:HB	1:B:924:GLN:HE21	1.80	0.46
1:C:403:PRO:HA	3:C:2002:PLM:H62	1.97	0.46
1:C:722:ASP:OD1	1:C:722:ASP:N	2.48	0.46
1:B:73:ASN:HB2	1:B:337:VAL:HG12	1.97	0.46
1:B:112:TYR:HB2	1:B:305:PRO:HG3	1.96	0.46
1:B:492:VAL:HA	1:B:493:PRO:HD3	1.75	0.46
1:B:1082:GLN:HE22	1:B:1085:ARG:HH11	1.64	0.46
1:A:912:GLN:OE1	1:A:913:GLY:N	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:GLN:HB3	1:A:854:ASN:H	1.49	0.46
1:B:712:MET:HE3	1:B:712:MET:HB3	1.79	0.46
1:A:202:ASN:OD1	1:A:202:ASN:N	2.49	0.46
1:B:1039:ASN:HD22	1:B:1041:PHE:H	1.63	0.46
1:C:125:VAL:HG22	1:C:323:ILE:HG12	1.99	0.45
1:C:221:ASP:OD1	1:C:221:ASP:N	2.49	0.45
1:C:97:GLY:HA2	1:C:108:PHE:H	1.81	0.45
1:A:237:LYS:NZ	2:E:2:NAG:O7	2.36	0.45
1:A:402:PRO:C	3:A:3001:PLM:H91	2.42	0.45
1:C:458:THR:O	1:C:461:SER:HB3	2.16	0.45
1:A:402:PRO:HG3	1:A:408:LYS:HD2	1.98	0.45
1:B:351:ASP:OD1	1:B:351:ASP:N	2.46	0.45
1:B:534:SER:O	1:B:537:SER:OG	2.33	0.45
1:A:161:GLY:HA3	1:A:173:LEU:HD21	1.98	0.45
1:C:131:ALA:HA	1:C:147:ILE:HB	1.98	0.45
1:A:852:THR:O	1:A:852:THR:OG1	2.31	0.44
1:A:912:GLN:HB2	1:A:915:GLN:HG2	1.98	0.44
1:B:73:ASN:HA	1:B:335:PHE:O	2.17	0.44
1:B:100:ALA:HB3	1:B:103:ARG:HB2	1.99	0.44
1:A:95:SER:OG	1:A:96:ASP:O	2.35	0.44
1:B:496:LEU:H	1:B:496:LEU:HG	1.60	0.44
1:C:258:ASN:N	1:C:258:ASN:OD1	2.49	0.44
1:A:1176:SER:OG	1:A:1177:THR:N	2.50	0.44
1:C:73:ASN:HA	1:C:335:PHE:O	2.17	0.44
1:C:1152:LEU:HD22	1:C:1215:LEU:HD11	1.99	0.44
1:B:919:ASP:OD1	1:B:919:ASP:N	2.50	0.44
1:B:494:GLN:NE2	4:B:2008:NAG:H82	2.26	0.44
1:A:332:LEU:HB3	1:A:345:VAL:HB	1.99	0.44
1:A:455:ALA:HB3	3:A:3001:PLM:H61	2.00	0.43
1:C:69:LYS:HB3	1:C:69:LYS:HE2	1.81	0.43
1:C:823:GLN:H	1:C:823:GLN:HG3	1.49	0.43
1:B:313:ASN:OD1	1:B:313:ASN:N	2.35	0.43
1:C:1065:ASP:OD1	1:C:1069:ASN:ND2	2.50	0.43
1:B:168:ARG:HG3	1:B:209:PHE:HD2	1.84	0.43
1:B:221:ASP:OD1	1:B:221:ASP:N	2.51	0.43
1:C:875:GLN:HE21	1:C:875:GLN:HB2	1.53	0.43
1:C:384:GLU:OE1	1:C:639:TYR:OH	2.28	0.43
1:C:827:LYS:HA	1:C:827:LYS:HD3	1.86	0.43
1:A:46:SER:O	1:A:50:THR:OG1	2.29	0.43
1:C:1043:ALA:HB1	1:C:1063:GLN:HG3	2.00	0.43
1:A:804:LYS:HB3	1:A:804:LYS:HE2	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:PRO:HD3	3:B:2002:PLM:H91	2.00	0.43
1:B:804:LYS:HE2	1:B:804:LYS:HB3	1.76	0.43
1:C:334:ASN:ND2	1:C:342:THR:OG1	2.49	0.43
1:C:44:PHE:HA	1:C:138:VAL:HG11	2.01	0.42
1:A:653:VAL:HG21	1:C:910:MET:HE1	2.02	0.42
1:C:83:PRO:O	1:C:331:TYR:OH	2.34	0.42
1:B:660:ILE:O	1:B:668:HIS:HA	2.19	0.42
1:A:108:PHE:HD2	1:A:139:ILE:HD12	1.85	0.42
1:C:852:THR:O	1:C:852:THR:OG1	2.34	0.42
1:C:853:GLN:HB3	1:C:854:ASN:H	1.45	0.42
1:A:774:GLY:HA3	1:A:1148:ALA:O	2.19	0.42
1:B:182:ASP:OD1	1:B:183:GLY:N	2.51	0.42
1:A:354:GLN:HE22	1:A:372:SER:H	1.68	0.42
1:A:502:PRO:HG3	3:A:3001:PLM:C8	2.49	0.42
1:C:853:GLN:O	1:C:854:ASN:ND2	2.51	0.42
1:B:1208:MET:HE3	1:B:1208:MET:HB3	1.93	0.42
1:B:962:SER:HB3	1:C:1140:PRO:HG3	2.02	0.42
1:A:594:ILE:HD12	1:A:594:ILE:HA	1.92	0.41
1:B:809:ASN:HD21	1:B:1071:ARG:HH12	1.68	0.41
1:C:867:ASN:OD1	1:C:869:THR:OG1	2.31	0.41
1:B:506:ALA:HA	1:B:557:TYR:O	2.18	0.41
1:C:96:ASP:OD1	1:C:97:GLY:N	2.53	0.41
1:C:152:PRO:HB3	1:C:321:PHE:CZ	2.56	0.41
1:B:366:THR:HG22	1:B:726:LEU:HD21	2.02	0.41
1:C:260:GLU:OE2	1:C:276:SER:OG	2.39	0.41
1:C:351:ASP:OD1	1:C:351:ASP:N	2.46	0.41
1:C:402:PRO:HG3	1:C:408:LYS:HD2	2.03	0.41
1:B:502:PRO:HB3	3:B:2002:PLM:HA1	2.03	0.41
1:C:496:LEU:N	1:C:496:LEU:CD1	2.84	0.41
1:C:383:ILE:H	1:C:383:ILE:HG13	1.54	0.41
1:A:171:ARG:HD3	1:A:173:LEU:HD23	2.03	0.41
1:B:69:LYS:HB3	1:B:69:LYS:HE2	1.89	0.41
1:C:391:CYS:SG	1:C:417:TYR:HB3	2.61	0.41
1:A:256:ASP:OD2	1:A:258:ASN:ND2	2.54	0.41
1:B:735:ILE:HA	1:B:736:PRO:HD3	1.93	0.41
1:B:813:LYS:H	1:B:813:LYS:HG2	1.62	0.41
1:B:1109:LYS:HD3	1:B:1109:LYS:HA	1.68	0.41
1:C:712:MET:HE3	1:C:712:MET:HB3	1.95	0.41
1:C:735:ILE:HA	1:C:736:PRO:HD3	1.85	0.41
1:C:766:THR:O	1:C:766:THR:OG1	2.32	0.41
1:B:94:PHE:HD2	1:B:150:ILE:HG21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASN:HD22	1:A:174:ASN:HA	1.80	0.40
1:A:401:PRO:HG2	1:A:565:LEU:HD21	2.03	0.40
1:C:506:ALA:HA	1:C:557:TYR:O	2.21	0.40
1:A:660:ILE:O	1:A:668:HIS:HA	2.21	0.40
1:B:83:PRO:O	1:B:331:TYR:OH	2.28	0.40
1:B:971:GLN:HG2	1:C:1211:LYS:HE2	2.03	0.40
1:B:168:ARG:NH2	1:B:209:PHE:O	2.55	0.40
1:C:796:ILE:H	1:C:839:GLN:NE2	2.20	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	1157/1352 (86%)	1082 (94%)	69 (6%)	6 (0%)	25	38
1	B	1157/1352 (86%)	1086 (94%)	64 (6%)	7 (1%)	22	33
1	C	1157/1352 (86%)	1077 (93%)	74 (6%)	6 (0%)	25	38
All	All	3471/4056 (86%)	3245 (94%)	207 (6%)	19 (0%)	27	38

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	ILE
1	A	853	GLN
1	A	854	ASN
1	B	383	ILE
1	B	853	GLN
1	C	853	GLN
1	C	854	ASN
1	B	854	ASN
1	C	383	ILE

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Mol	Chain	Res	Type
1	A	174	ASN
1	A	137	THR
1	B	590	ASN
1	C	590	ASN
1	B	174	ASN
1	B	764	PRO
1	C	137	THR
1	C	174	ASN
1	A	138	VAL
1	B	138	VAL

5.3.2 Protein sidechains [i](#)

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	1004/1174 (86%)	903 (90%)	101 (10%)	6	9
1	B	1004/1174 (86%)	910 (91%)	94 (9%)	7	11
1	C	1004/1174 (86%)	894 (89%)	110 (11%)	5	7
All	All	3012/3522 (86%)	2707 (90%)	305 (10%)	9	9

All (305) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	47	VAL
1	A	49	THR
1	A	51	TRP
1	A	58	SER
1	A	67	ASN
1	A	76	LEU
1	A	93	LEU
1	A	95	SER
1	A	108	PHE
1	A	133	LYS
1	A	137	THR

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Mol	Chain	Res	Type
1	A	139	ILE
1	A	160	VAL
1	A	173	LEU
1	A	180	LEU
1	A	184	CYS
1	A	202	ASN
1	A	210	LYS
1	A	212	LEU
1	A	230	GLU
1	A	232	THR
1	A	246	THR
1	A	268	THR
1	A	278	LYS
1	A	280	ASN
1	A	296	GLN
1	A	307	SER
1	A	315	ARG
1	A	364	VAL
1	A	375	GLU
1	A	389	GLN
1	A	390	GLU
1	A	394	THR
1	A	408	LYS
1	A	421	LYS
1	A	427	GLN
1	A	441	LEU
1	A	446	TYR
1	A	492	VAL
1	A	494	GLN
1	A	496	LEU
1	A	497	THR
1	A	503	SER
1	A	513	LYS
1	A	530	THR
1	A	542	THR
1	A	579	THR
1	A	581	SER
1	A	591	ASP
1	A	592	THR
1	A	593	SER
1	A	594	ILE
1	A	597	LYS

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Mol	Chain	Res	Type
1	A	624	ARG
1	A	634	ASP
1	A	659	VAL
1	A	667	SER
1	A	720	VAL
1	A	723	GLU
1	A	773	THR
1	A	776	VAL
1	A	805	GLN
1	A	813	LYS
1	A	818	LEU
1	A	827	LYS
1	A	837	LEU
1	A	839	GLN
1	A	848	SER
1	A	852	THR
1	A	855	THR
1	A	858	LEU
1	A	862	LEU
1	A	870	MET
1	A	884	ARG
1	A	890	LEU
1	A	895	VAL
1	A	904	GLN
1	A	912	GLN
1	A	918	ARG
1	A	948	LEU
1	A	958	THR
1	A	967	ILE
1	A	971	GLN
1	A	991	GLN
1	A	992	LYS
1	A	1006	GLN
1	A	1039	ASN
1	A	1061	GLU
1	A	1063	GLN
1	A	1065	ASP
1	A	1106	SER
1	A	1139	GLN
1	A	1154	ASN
1	A	1156	GLU
1	A	1171	LEU

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Mol	Chain	Res	Type
1	A	1173	GLN
1	A	1177	THR
1	A	1180	ASP
1	A	1223	LEU
1	A	1224	LEU
1	B	40	GLN
1	B	45	GLU
1	B	47	VAL
1	B	50	THR
1	B	51	TRP
1	B	67	ASN
1	B	93	LEU
1	B	95	SER
1	B	98	HIS
1	B	108	PHE
1	B	114	SER
1	B	117	GLU
1	B	133	LYS
1	B	136	THR
1	B	137	THR
1	B	139	ILE
1	B	160	VAL
1	B	163	TYR
1	B	169	THR
1	B	173	LEU
1	B	202	ASN
1	B	207	THR
1	B	221	ASP
1	B	229	GLN
1	B	230	GLU
1	B	268	THR
1	B	278	LYS
1	B	309	ARG
1	B	313	ASN
1	B	337	VAL
1	B	379	ARG
1	B	389	GLN
1	B	390	GLU
1	B	408	LYS
1	B	421	LYS
1	B	441	LEU
1	B	446	TYR

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Mol	Chain	Res	Type
1	B	482	SER
1	B	492	VAL
1	B	494	GLN
1	B	496	LEU
1	B	503	SER
1	B	513	LYS
1	B	514	THR
1	B	515	SER
1	B	570	ILE
1	B	579	THR
1	B	581	SER
1	B	591	ASP
1	B	592	THR
1	B	619	THR
1	B	627	ARG
1	B	650	ARG
1	B	665	SER
1	B	683	MET
1	B	704	LEU
1	B	723	GLU
1	B	738	THR
1	B	790	GLU
1	B	795	THR
1	B	805	GLN
1	B	813	LYS
1	B	818	LEU
1	B	819	LYS
1	B	820	GLU
1	B	823	GLN
1	B	837	LEU
1	B	848	SER
1	B	855	THR
1	B	858	LEU
1	B	862	LEU
1	B	865	ASP
1	B	869	THR
1	B	875	GLN
1	B	904	GLN
1	B	911	GLN
1	B	912	GLN
1	B	962	SER
1	B	967	ILE

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Mol	Chain	Res	Type
1	B	1006	GLN
1	B	1007	THR
1	B	1049	SER
1	B	1061	GLU
1	B	1063	GLN
1	B	1065	ASP
1	B	1092	SER
1	B	1107	GLN
1	B	1144	VAL
1	B	1171	LEU
1	B	1173	GLN
1	B	1177	THR
1	B	1182	ASP
1	B	1223	LEU
1	B	1224	LEU
1	C	40	GLN
1	C	42	ASP
1	C	45	GLU
1	C	46	SER
1	C	47	VAL
1	C	50	THR
1	C	51	TRP
1	C	67	ASN
1	C	93	LEU
1	C	108	PHE
1	C	117	GLU
1	C	121	ASP
1	C	133	LYS
1	C	137	THR
1	C	138	VAL
1	C	163	TYR
1	C	166	SER
1	C	173	LEU
1	C	184	CYS
1	C	199	THR
1	C	212	LEU
1	C	221	ASP
1	C	223	VAL
1	C	230	GLU
1	C	232	THR
1	C	246	THR
1	C	256	ASP

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Mol	Chain	Res	Type
1	C	258	ASN
1	C	268	THR
1	C	278	LYS
1	C	302	THR
1	C	308	ILE
1	C	364	VAL
1	C	375	GLU
1	C	379	ARG
1	C	389	GLN
1	C	390	GLU
1	C	408	LYS
1	C	421	LYS
1	C	430	GLU
1	C	441	LEU
1	C	446	TYR
1	C	492	VAL
1	C	494	GLN
1	C	495	ASN
1	C	498	THR
1	C	513	LYS
1	C	515	SER
1	C	534	SER
1	C	542	THR
1	C	552	LEU
1	C	570	ILE
1	C	581	SER
1	C	591	ASP
1	C	592	THR
1	C	596	ASP
1	C	619	THR
1	C	634	ASP
1	C	654	SER
1	C	683	MET
1	C	723	GLU
1	C	752	ASP
1	C	756	ILE
1	C	766	THR
1	C	790	GLU
1	C	795	THR
1	C	805	GLN
1	C	809	ASN
1	C	813	LYS

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Mol	Chain	Res	Type
1	C	818	LEU
1	C	820	GLU
1	C	823	GLN
1	C	837	LEU
1	C	848	SER
1	C	853	GLN
1	C	855	THR
1	C	862	LEU
1	C	875	GLN
1	C	878	THR
1	C	884	ARG
1	C	890	LEU
1	C	895	VAL
1	C	912	GLN
1	C	918	ARG
1	C	948	LEU
1	C	967	ILE
1	C	972	SER
1	C	991	GLN
1	C	1006	GLN
1	C	1031	SER
1	C	1033	LEU
1	C	1058	VAL
1	C	1059	GLU
1	C	1061	GLU
1	C	1063	GLN
1	C	1065	ASP
1	C	1081	GLN
1	C	1084	VAL
1	C	1087	GLU
1	C	1106	SER
1	C	1107	GLN
1	C	1144	VAL
1	C	1154	ASN
1	C	1156	GLU
1	C	1171	LEU
1	C	1182	ASP
1	C	1196	GLU
1	C	1223	LEU
1	C	1224	LEU
1	C	1228	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	98	HIS
1	A	141	GLN
1	A	269	GLN
1	A	285	ASN
1	A	354	GLN
1	A	389	GLN
1	A	414	ASN
1	A	494	GLN
1	A	504	ASN
1	A	616	HIS
1	A	679	HIS
1	A	755	GLN
1	A	809	ASN
1	A	853	GLN
1	A	856	GLN
1	A	875	GLN
1	A	904	GLN
1	A	911	GLN
1	A	1006	GLN
1	A	1039	ASN
1	A	1063	GLN
1	A	1082	GLN
1	A	1154	ASN
1	A	1173	GLN
1	A	1183	GLN
1	A	1184	GLN
1	A	1217	ASN
1	B	86	ASN
1	B	141	GLN
1	B	175	HIS
1	B	258	ASN
1	B	280	ASN
1	B	285	ASN
1	B	296	GLN
1	B	327	HIS
1	B	354	GLN
1	B	385	GLN
1	B	389	GLN
1	B	414	ASN
1	B	416	ASN
1	B	494	GLN

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Mol	Chain	Res	Type
1	B	524	ASN
1	B	626	GLN
1	B	645	ASN
1	B	666	ASN
1	B	809	ASN
1	B	875	GLN
1	B	904	GLN
1	B	911	GLN
1	B	915	GLN
1	B	924	GLN
1	B	1006	GLN
1	B	1039	ASN
1	B	1063	GLN
1	B	1081	GLN
1	B	1082	GLN
1	B	1129	ASN
1	B	1143	HIS
1	B	1154	ASN
1	B	1159	GLN
1	B	1173	GLN
1	B	1183	GLN
1	B	1226	ASN
1	C	48	HIS
1	C	141	GLN
1	C	288	HIS
1	C	334	ASN
1	C	354	GLN
1	C	385	GLN
1	C	414	ASN
1	C	504	ASN
1	C	616	HIS
1	C	640	HIS
1	C	666	ASN
1	C	755	GLN
1	C	809	ASN
1	C	839	GLN
1	C	853	GLN
1	C	856	GLN
1	C	875	GLN
1	C	904	GLN
1	C	911	GLN
1	C	915	GLN

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Mol	Chain	Res	Type
1	C	990	ASN
1	C	1006	GLN
1	C	1039	ASN
1	C	1063	GLN
1	C	1081	GLN
1	C	1082	GLN
1	C	1097	GLN
1	C	1154	ASN
1	C	1173	GLN
1	C	1183	GLN
1	C	1226	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 ⓘ

48 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	0.34	0	17,19,21	0.67	1 (5%)
2	NAG	D	2	2	14,14,15	0.32	0	17,19,21	0.48	0
2	NAG	E	1	1,2	14,14,15	0.21	0	17,19,21	0.64	0
2	NAG	E	2	2	14,14,15	0.36	0	17,19,21	0.59	0
2	NAG	F	1	1,2	14,14,15	0.40	0	17,19,21	0.61	0
2	NAG	F	2	2	14,14,15	0.40	0	17,19,21	0.56	0
2	NAG	G	1	1,2	14,14,15	0.27	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	G	2	2	14,14,15	0.31	0	17,19,21	0.55	0
2	NAG	H	1	1,2	14,14,15	0.33	0	17,19,21	0.62	0
2	NAG	H	2	2	14,14,15	0.21	0	17,19,21	0.50	0
2	NAG	I	1	1,2	14,14,15	0.31	0	17,19,21	0.68	1 (5%)
2	NAG	I	2	2	14,14,15	0.41	0	17,19,21	0.57	0
2	NAG	J	1	1,2	14,14,15	0.26	0	17,19,21	0.37	0
2	NAG	J	2	2	14,14,15	0.39	0	17,19,21	0.58	0
2	NAG	K	1	1,2	14,14,15	0.24	0	17,19,21	0.50	0
2	NAG	K	2	2	14,14,15	0.27	0	17,19,21	0.82	1 (5%)
2	NAG	L	1	1,2	14,14,15	0.81	1 (7%)	17,19,21	0.91	1 (5%)
2	NAG	L	2	2	14,14,15	0.42	0	17,19,21	0.38	0
2	NAG	M	1	1,2	14,14,15	0.21	0	17,19,21	0.57	0
2	NAG	M	2	2	14,14,15	0.42	0	17,19,21	0.58	0
2	NAG	N	1	1,2	14,14,15	0.46	0	17,19,21	0.69	1 (5%)
2	NAG	N	2	2	14,14,15	0.40	0	17,19,21	0.54	0
2	NAG	O	1	1,2	14,14,15	0.32	0	17,19,21	0.64	1 (5%)
2	NAG	O	2	2	14,14,15	0.41	0	17,19,21	0.52	0
2	NAG	P	1	1,2	14,14,15	0.47	0	17,19,21	0.63	0
2	NAG	P	2	2	14,14,15	0.26	0	17,19,21	0.59	0
2	NAG	Q	1	1,2	14,14,15	0.42	0	17,19,21	0.81	1 (5%)
2	NAG	Q	2	2	14,14,15	0.36	0	17,19,21	0.60	1 (5%)
2	NAG	R	1	1,2	14,14,15	0.25	0	17,19,21	0.57	0
2	NAG	R	2	2	14,14,15	0.26	0	17,19,21	0.59	0
2	NAG	S	1	1,2	14,14,15	0.41	0	17,19,21	0.61	0
2	NAG	S	2	2	14,14,15	0.33	0	17,19,21	0.63	1 (5%)
2	NAG	T	1	1,2	14,14,15	0.37	0	17,19,21	0.78	1 (5%)
2	NAG	T	2	2	14,14,15	0.40	0	17,19,21	0.37	0
2	NAG	U	1	1,2	14,14,15	0.28	0	17,19,21	0.50	0
2	NAG	U	2	2	14,14,15	0.30	0	17,19,21	0.57	0
2	NAG	V	1	1,2	14,14,15	0.56	0	17,19,21	0.58	0
2	NAG	V	2	2	14,14,15	0.46	0	17,19,21	0.60	0
2	NAG	W	1	1,2	14,14,15	0.34	0	17,19,21	0.69	1 (5%)
2	NAG	W	2	2	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	X	1	1,2	14,14,15	0.29	0	17,19,21	0.66	0
2	NAG	X	2	2	14,14,15	0.29	0	17,19,21	0.51	0
2	NAG	Y	1	1,2	14,14,15	0.26	0	17,19,21	0.62	1 (5%)
2	NAG	Y	2	2	14,14,15	0.25	0	17,19,21	0.60	0
2	NAG	Z	1	1,2	14,14,15	0.37	0	17,19,21	0.50	0
2	NAG	Z	2	2	14,14,15	0.38	0	17,19,21	0.54	0
2	NAG	a	1	1,2	14,14,15	0.25	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	a	2	2	14,14,15	0.22	0	17,19,21	0.68	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	-	1/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	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	-	2/6/23/26	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	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Y	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/23/26	0/1/1/1
2	NAG	a	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	a	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1	NAG	O5-C1	-2.86	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	1	NAG	C1-O5-C5	3.07	116.35	112.19
2	K	2	NAG	C1-O5-C5	3.00	116.26	112.19
2	L	1	NAG	C1-O5-C5	2.63	115.76	112.19
2	T	1	NAG	C1-O5-C5	2.58	115.68	112.19
2	a	2	NAG	C1-O5-C5	2.46	115.52	112.19
2	I	1	NAG	C1-O5-C5	2.38	115.41	112.19
2	N	1	NAG	C1-O5-C5	2.26	115.26	112.19
2	W	1	NAG	C1-O5-C5	2.26	115.25	112.19
2	S	2	NAG	C1-O5-C5	2.24	115.23	112.19
2	D	1	NAG	C1-O5-C5	2.18	115.14	112.19
2	Q	2	NAG	C1-O5-C5	2.12	115.07	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	NAG	C1-O5-C5	2.10	115.04	112.19
2	Y	1	NAG	C1-O5-C5	2.10	115.03	112.19

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	Z	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	Z	1	NAG	C4-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	V	1	NAG	C4-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	a	1	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	a	2	NAG	C4-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	U	2	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6

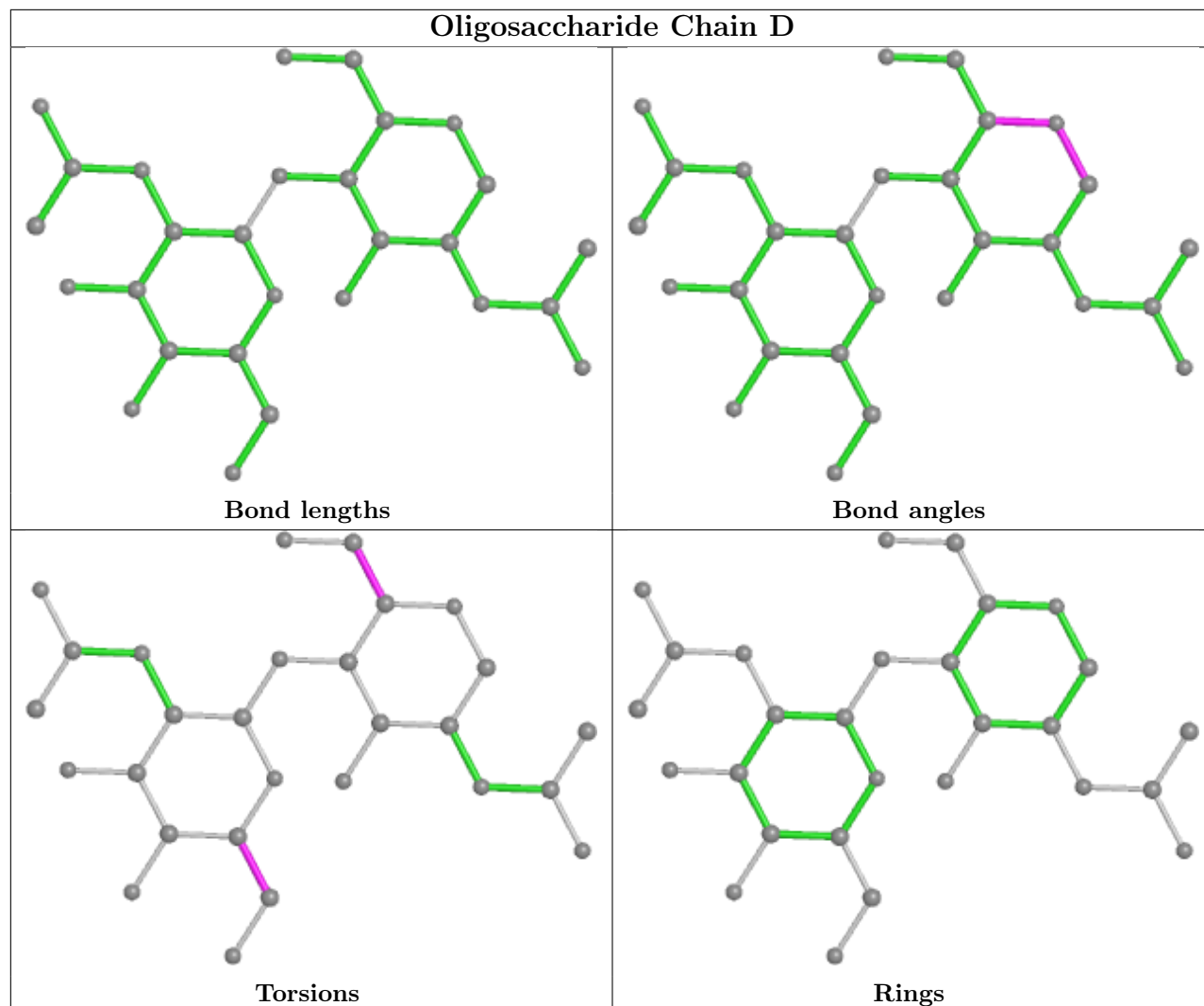
There are no ring outliers.

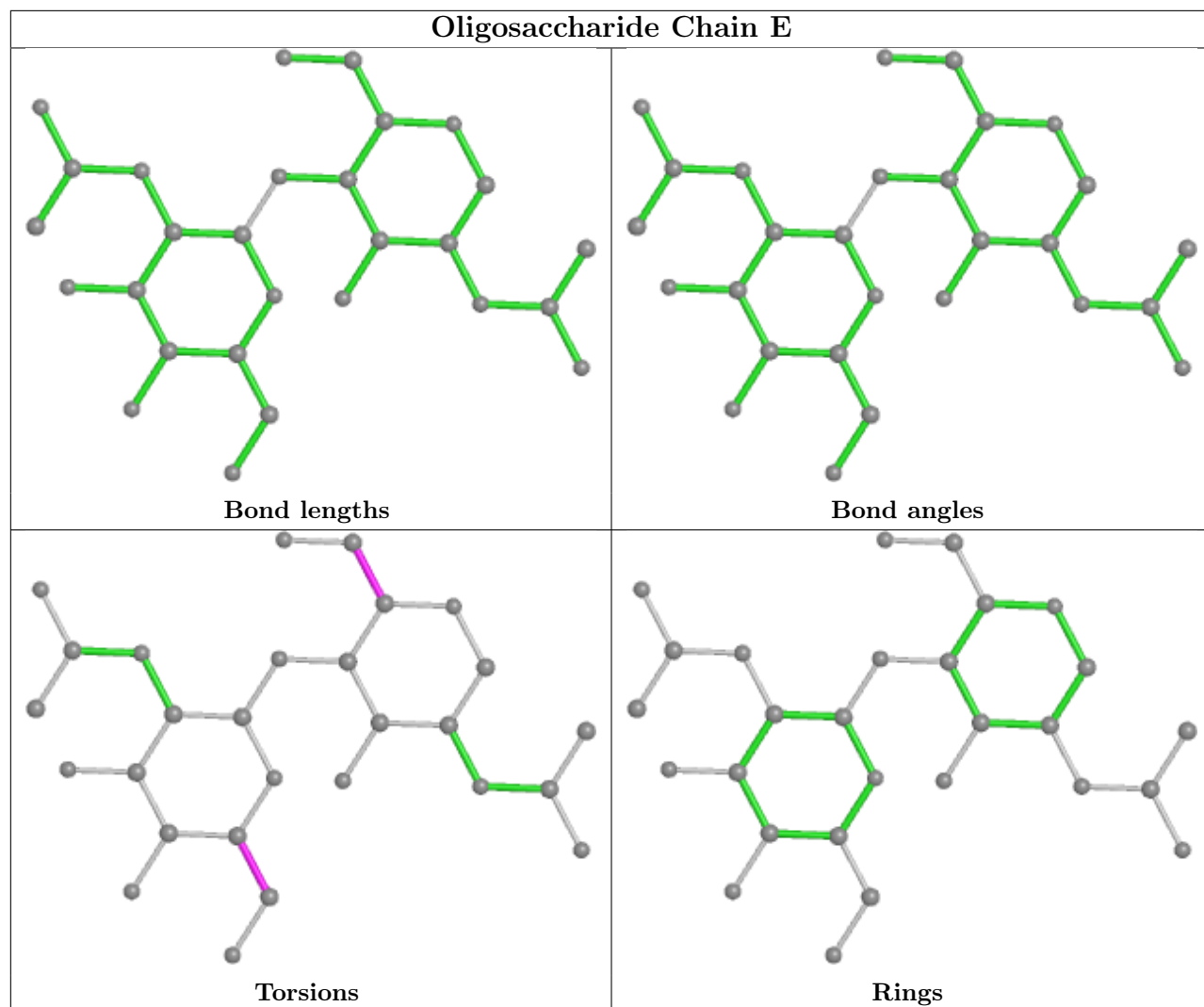
2 monomers are involved in 2 short contacts:

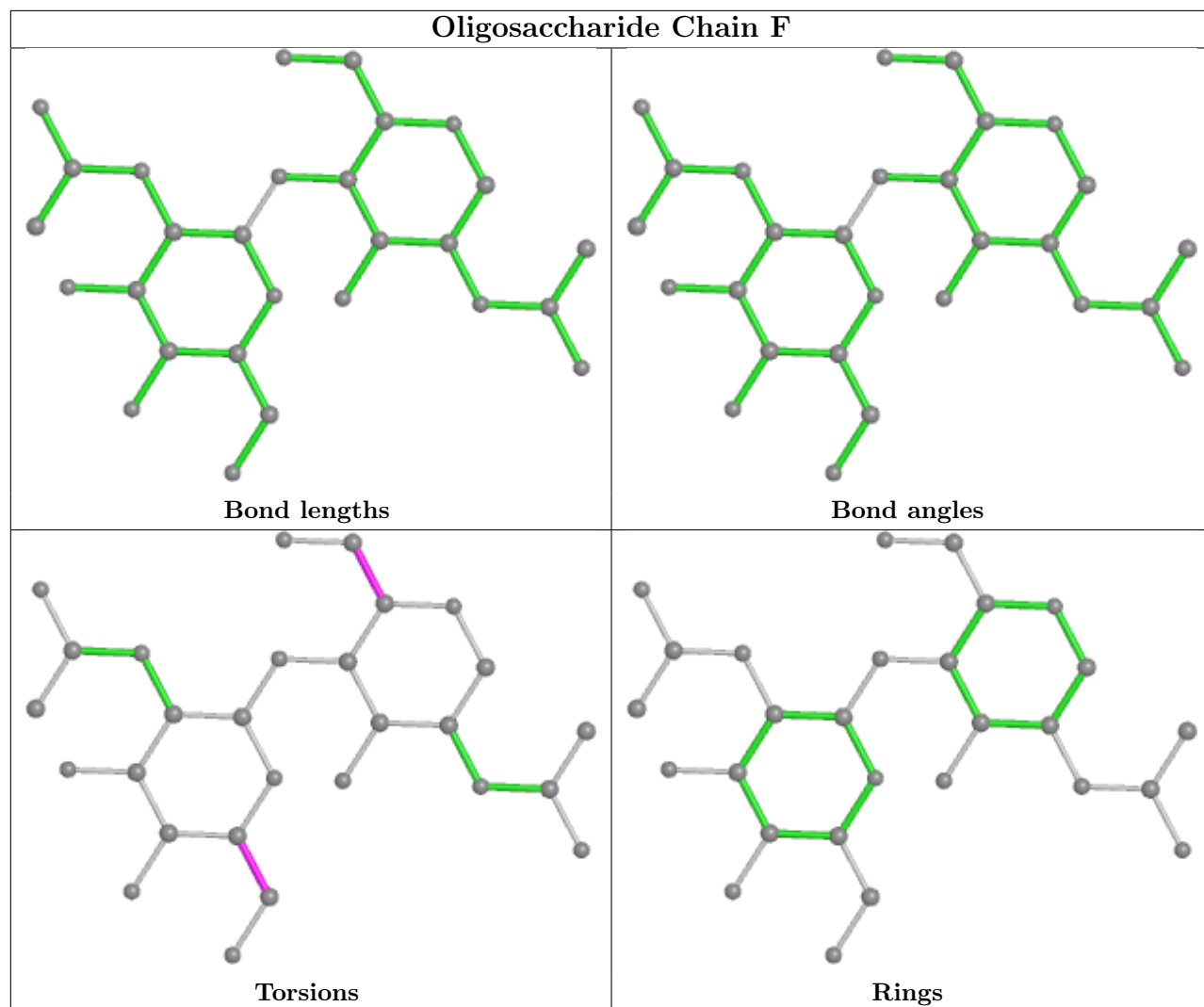
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	1	NAG	1	0
2	E	2	NAG	1	0

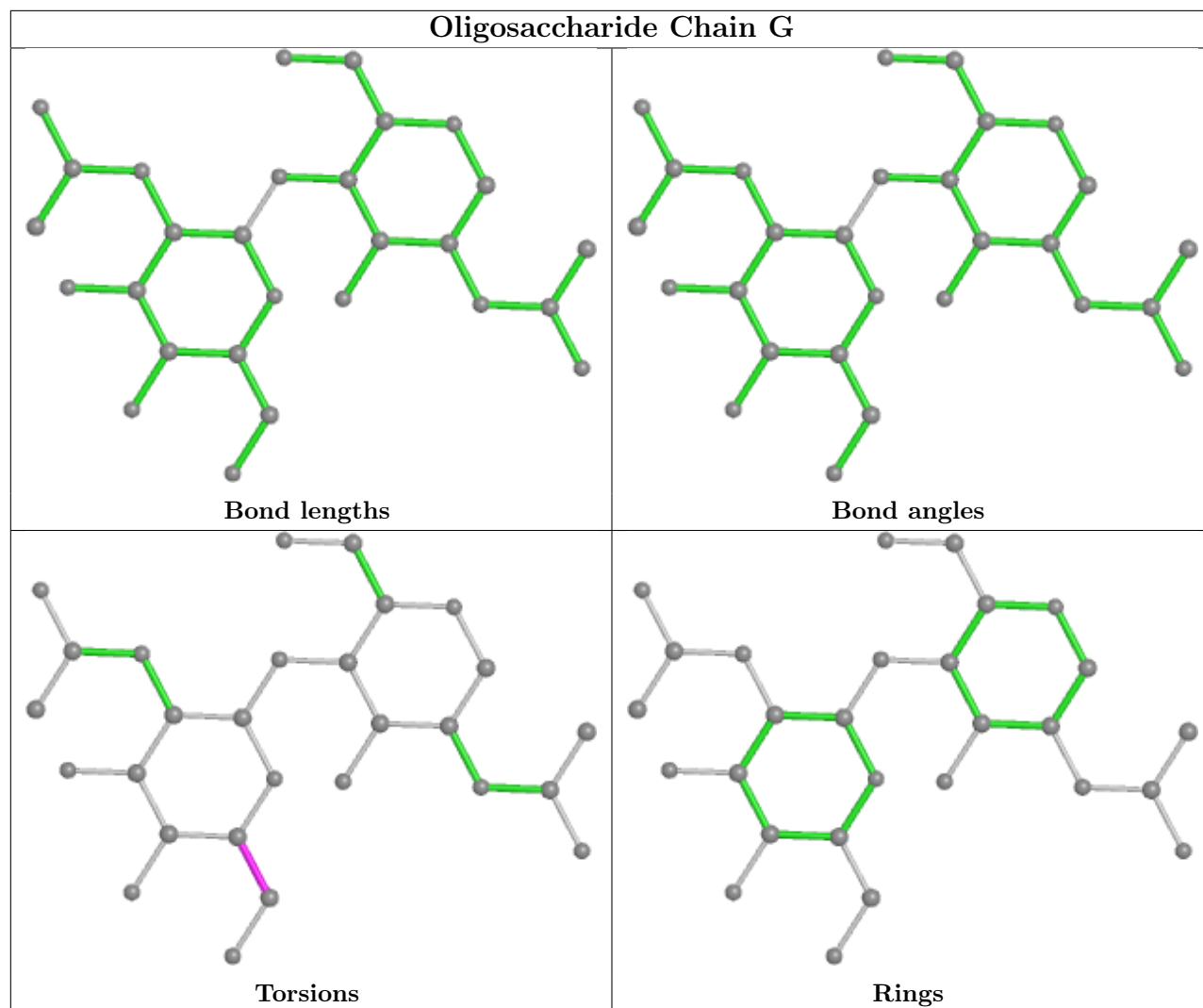
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

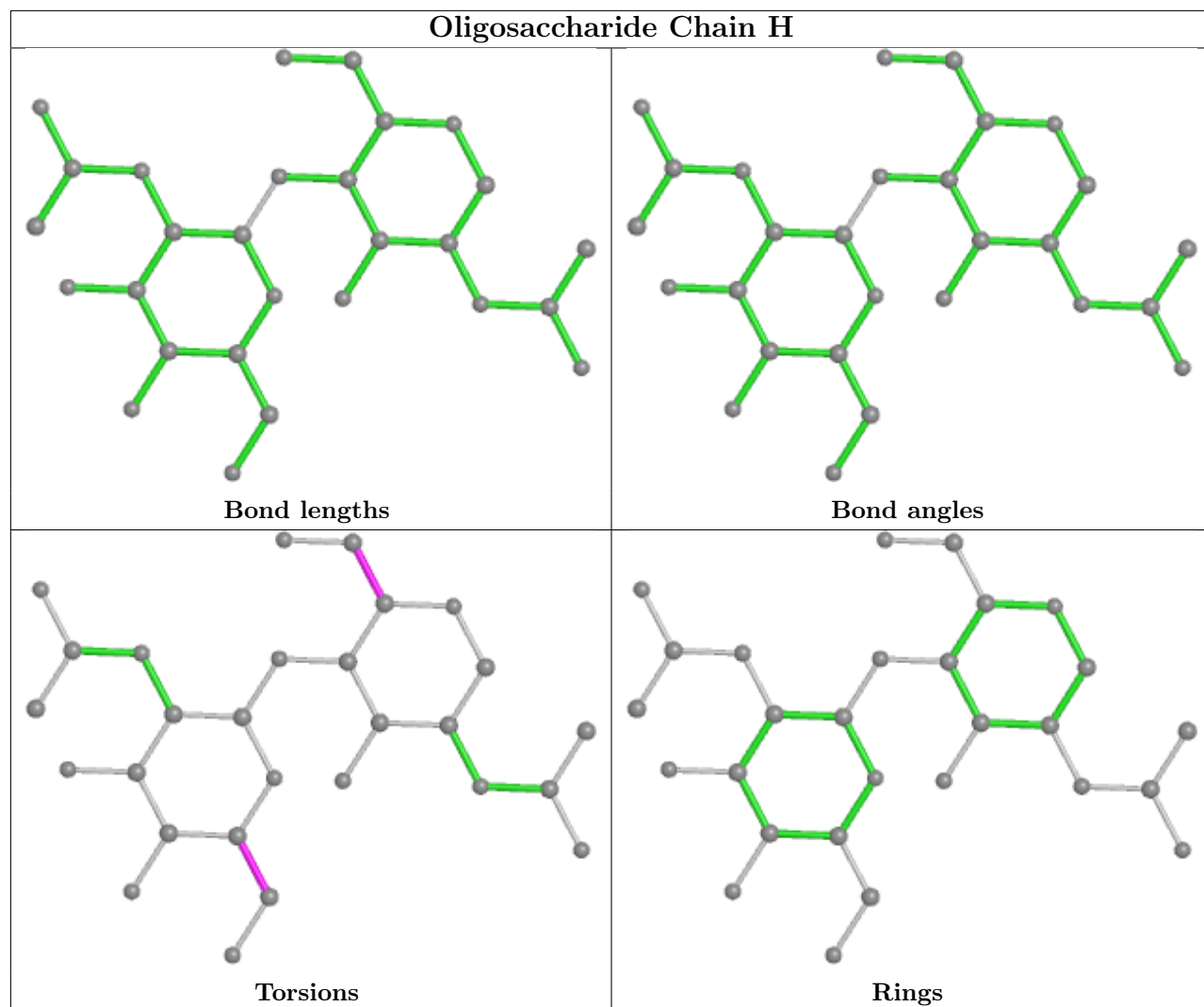
bond angles, torsion angles, and ring geometry for oligosaccharide.

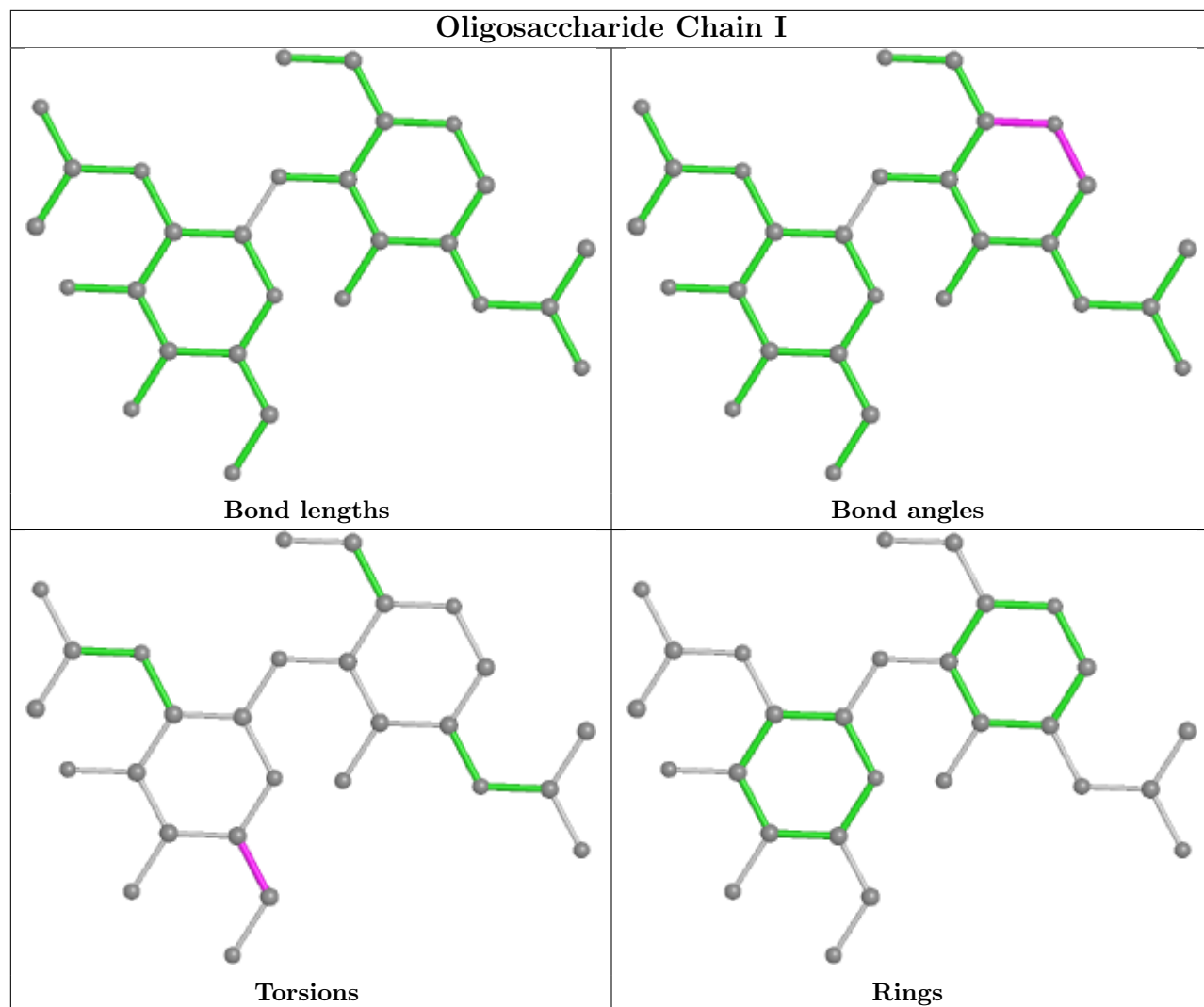


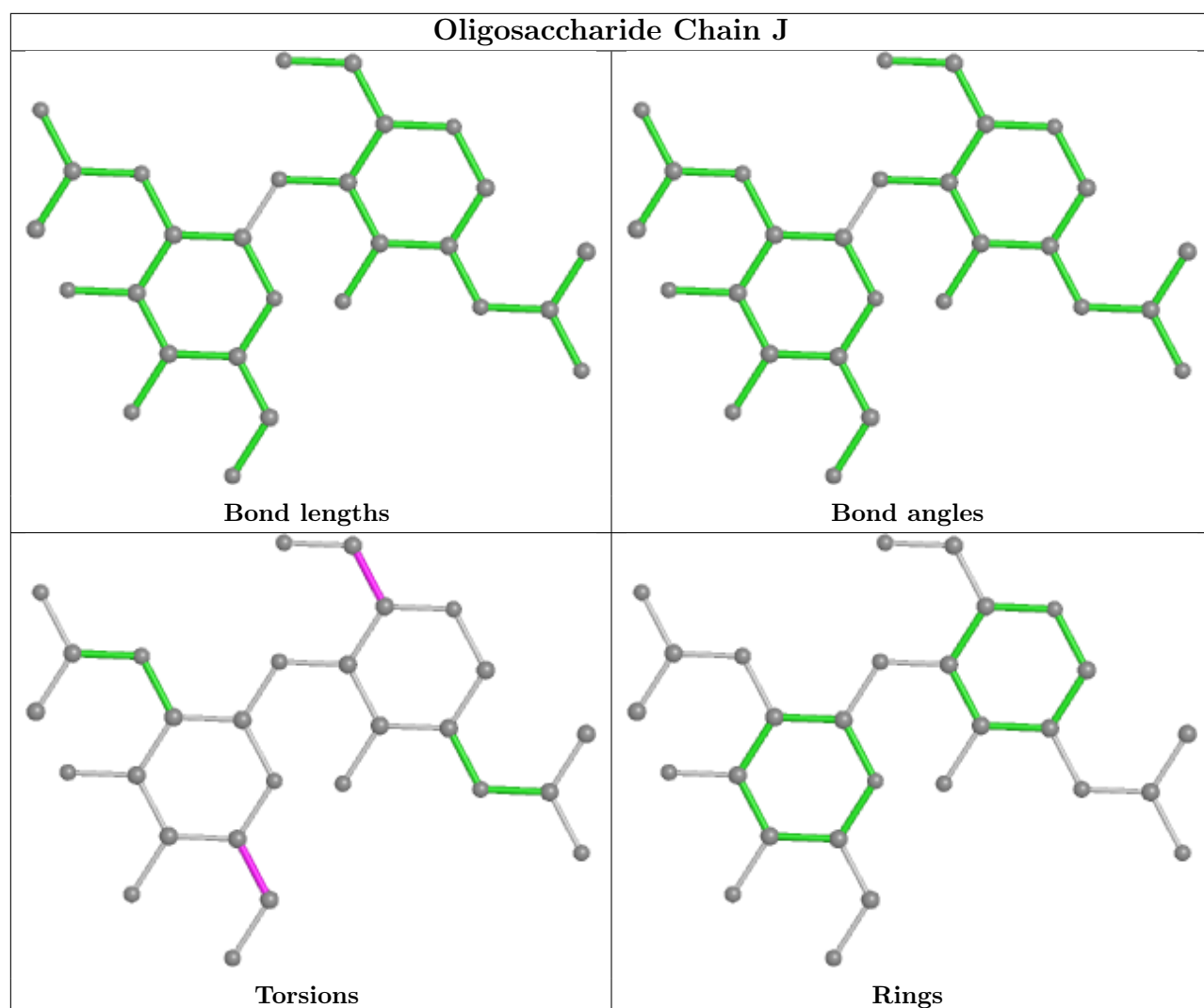


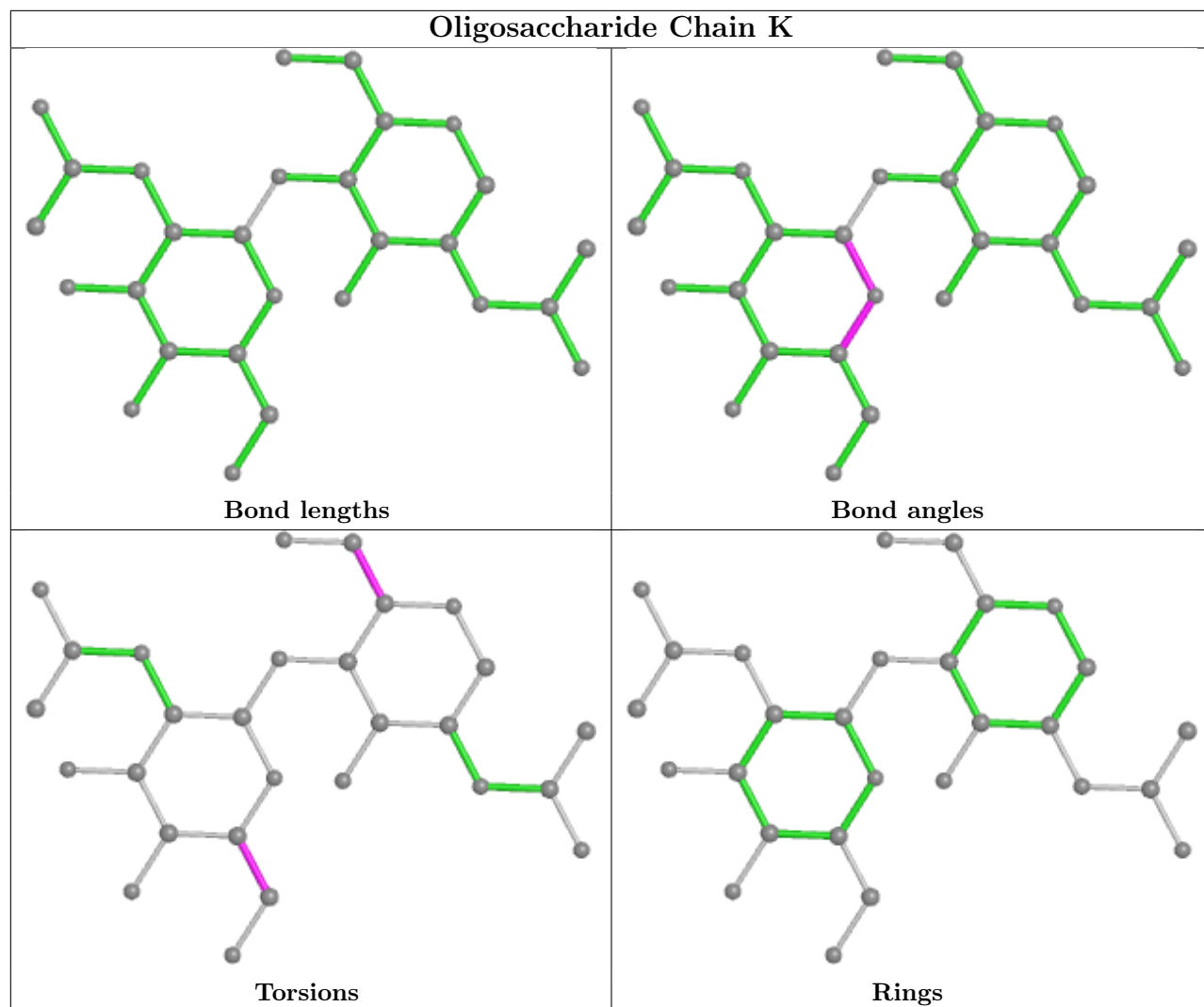


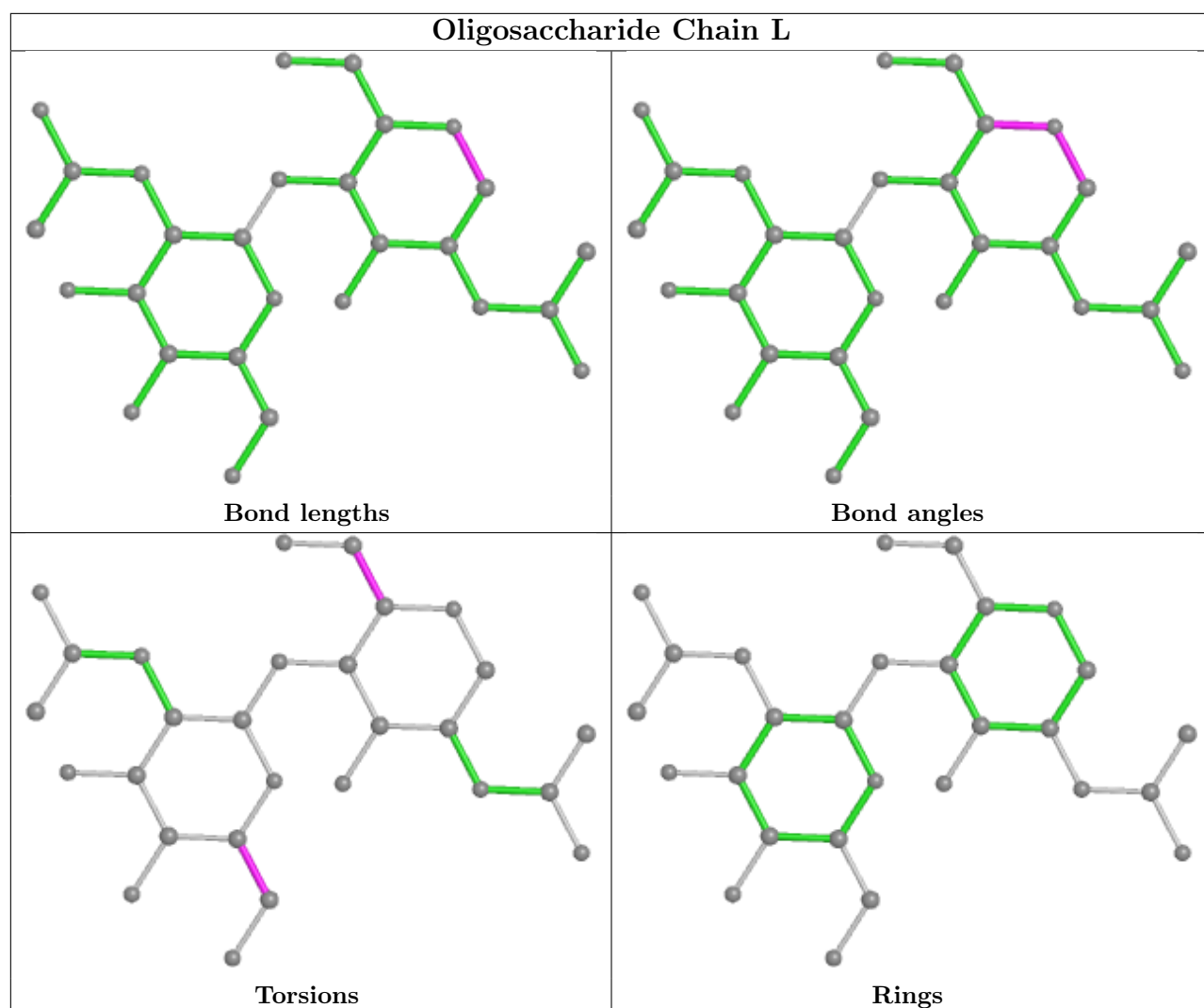


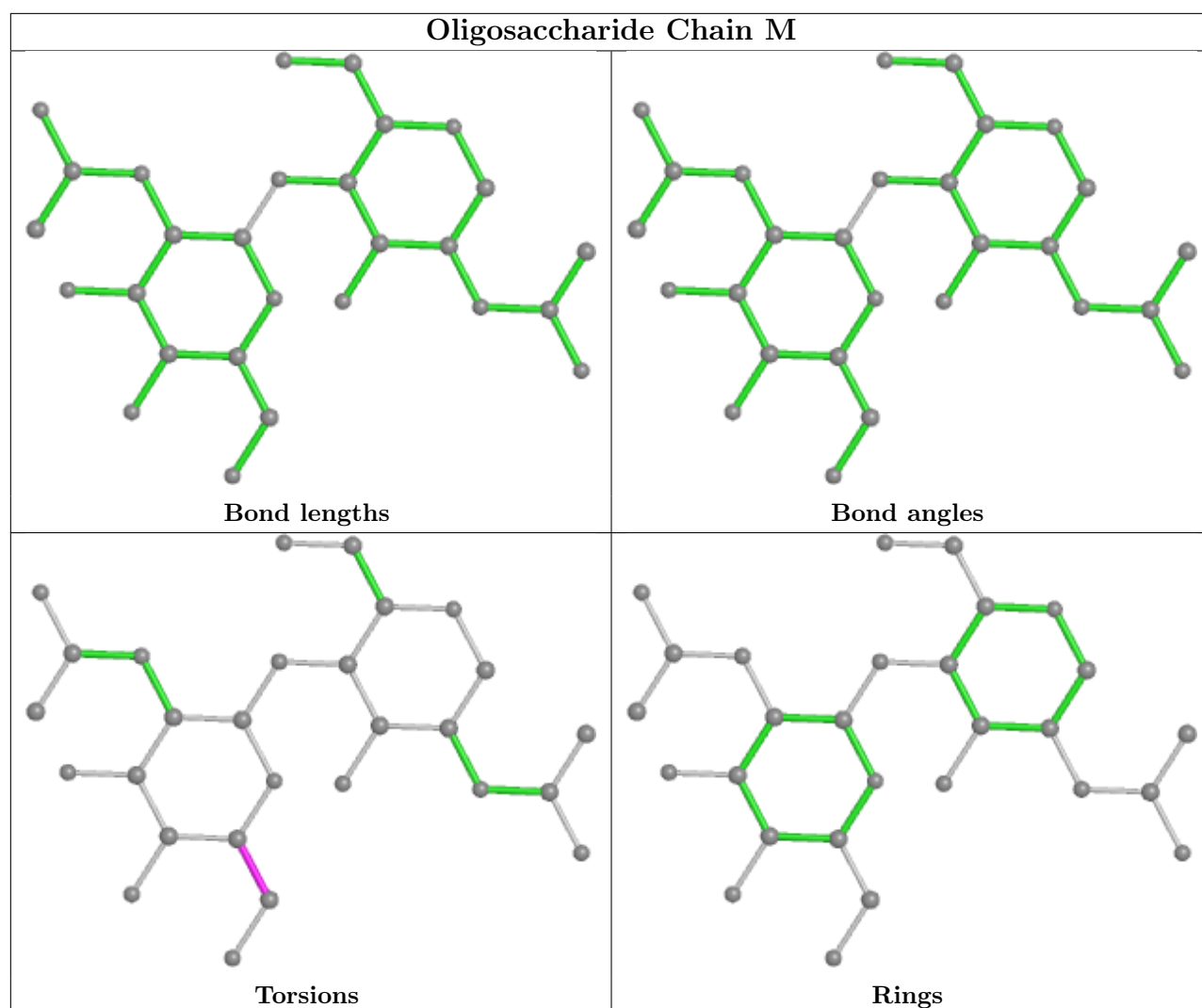


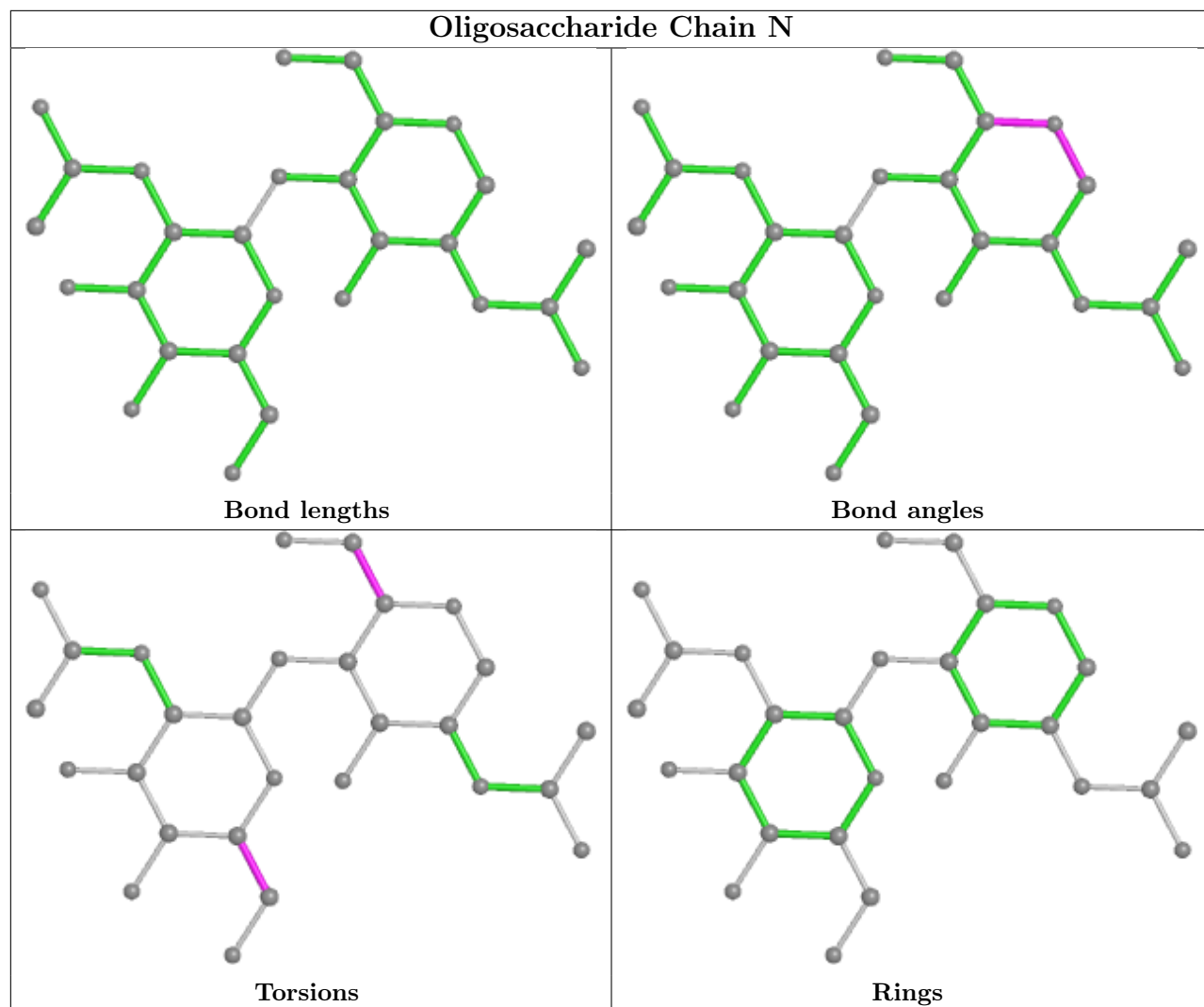


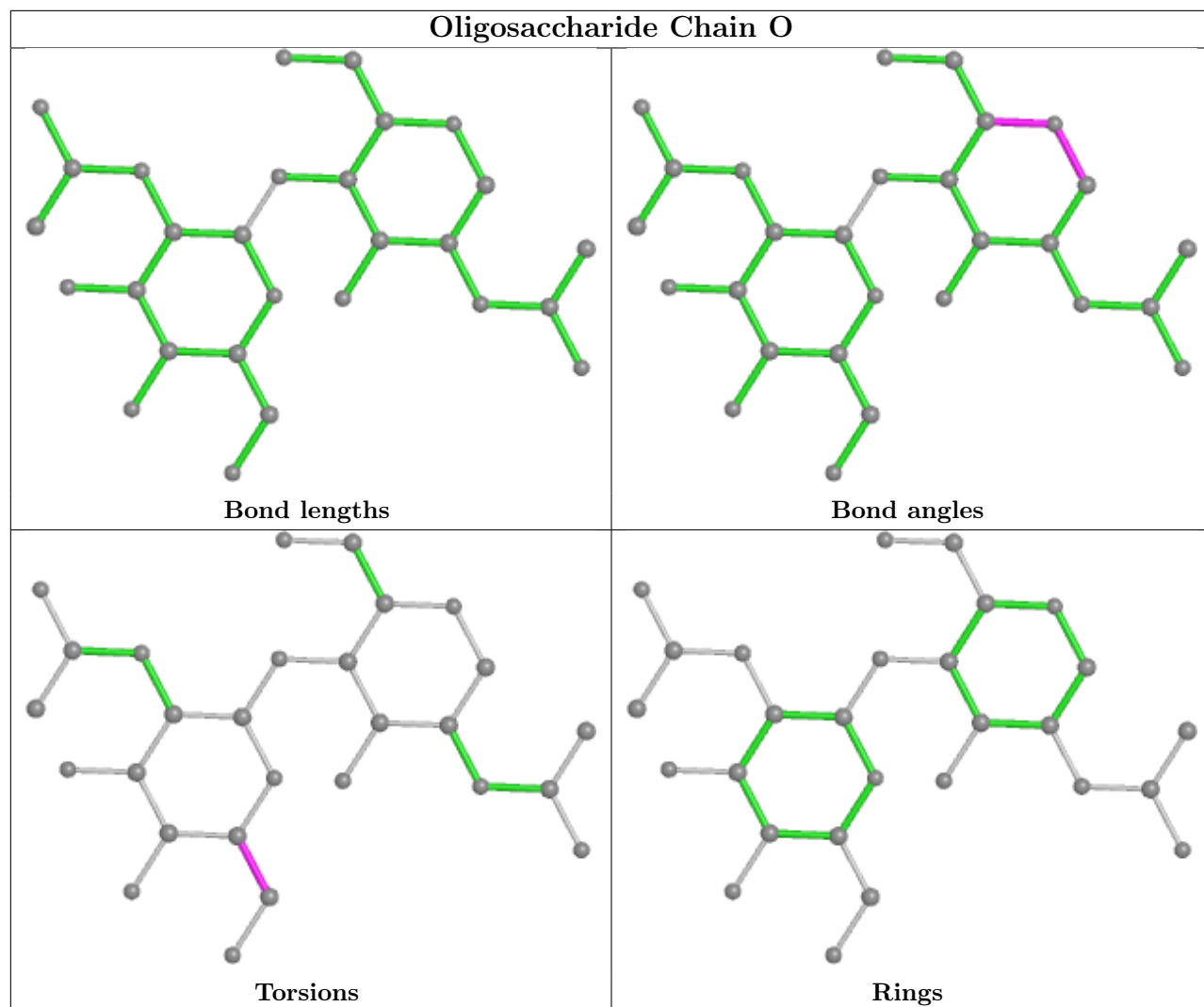


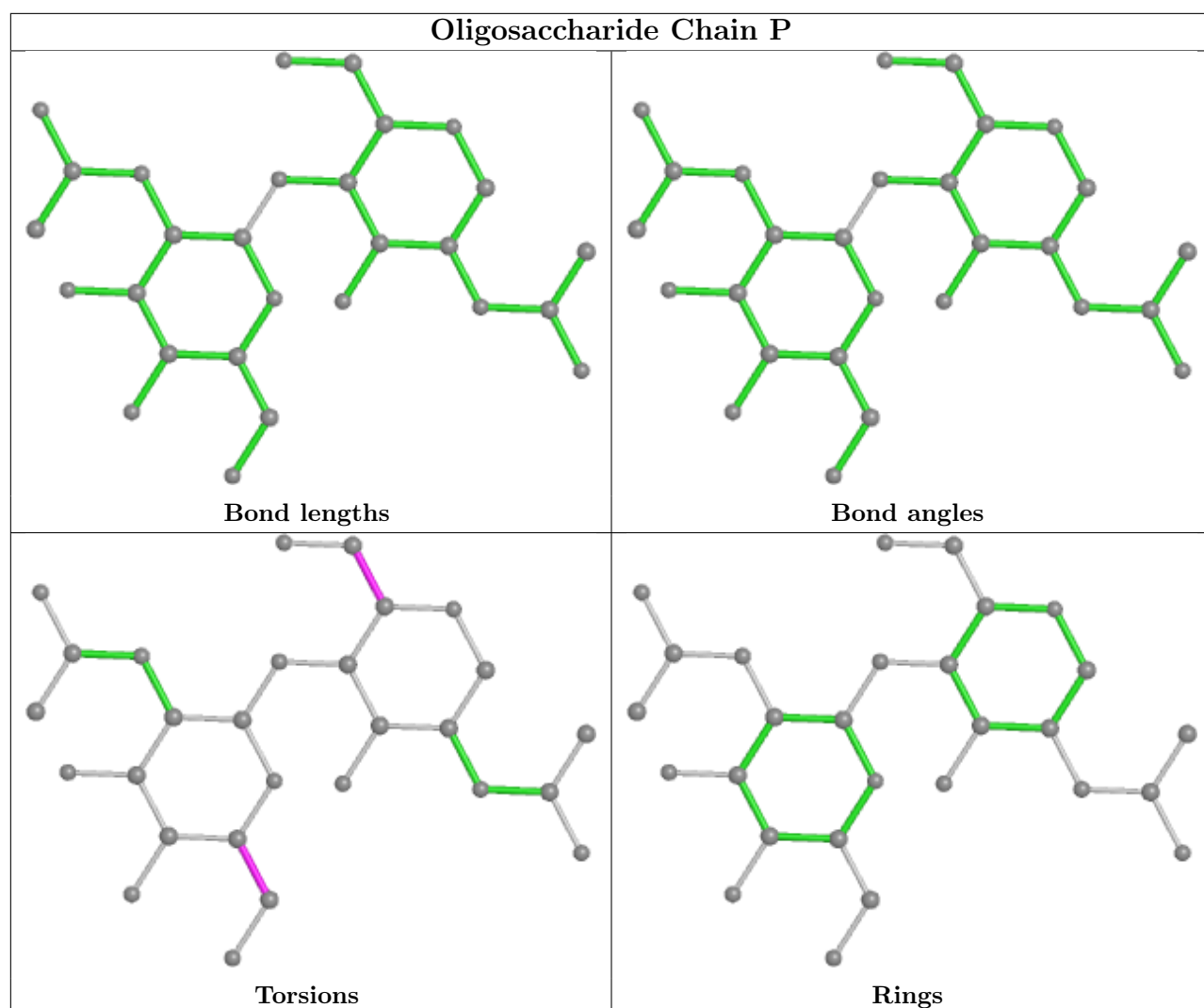


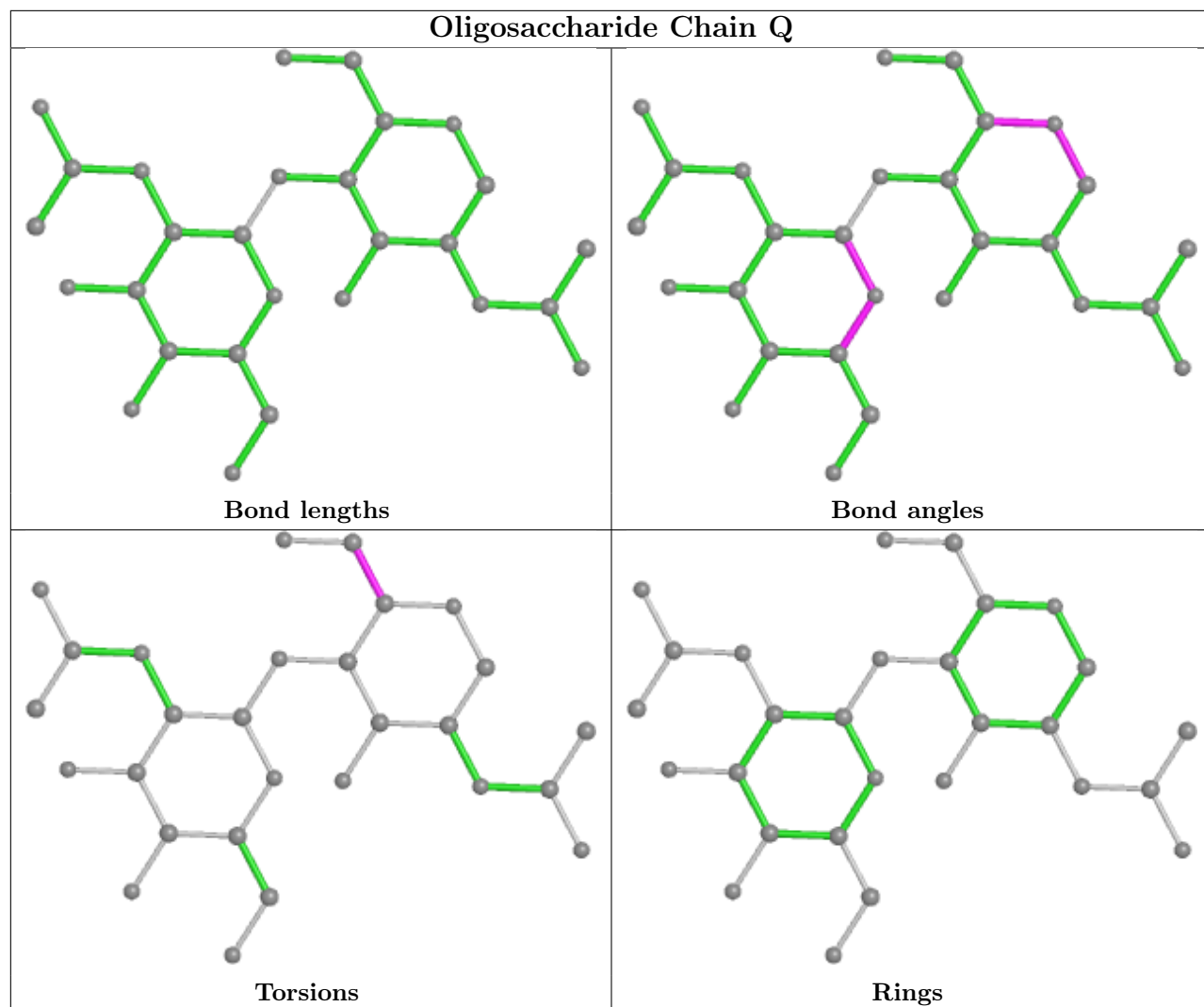


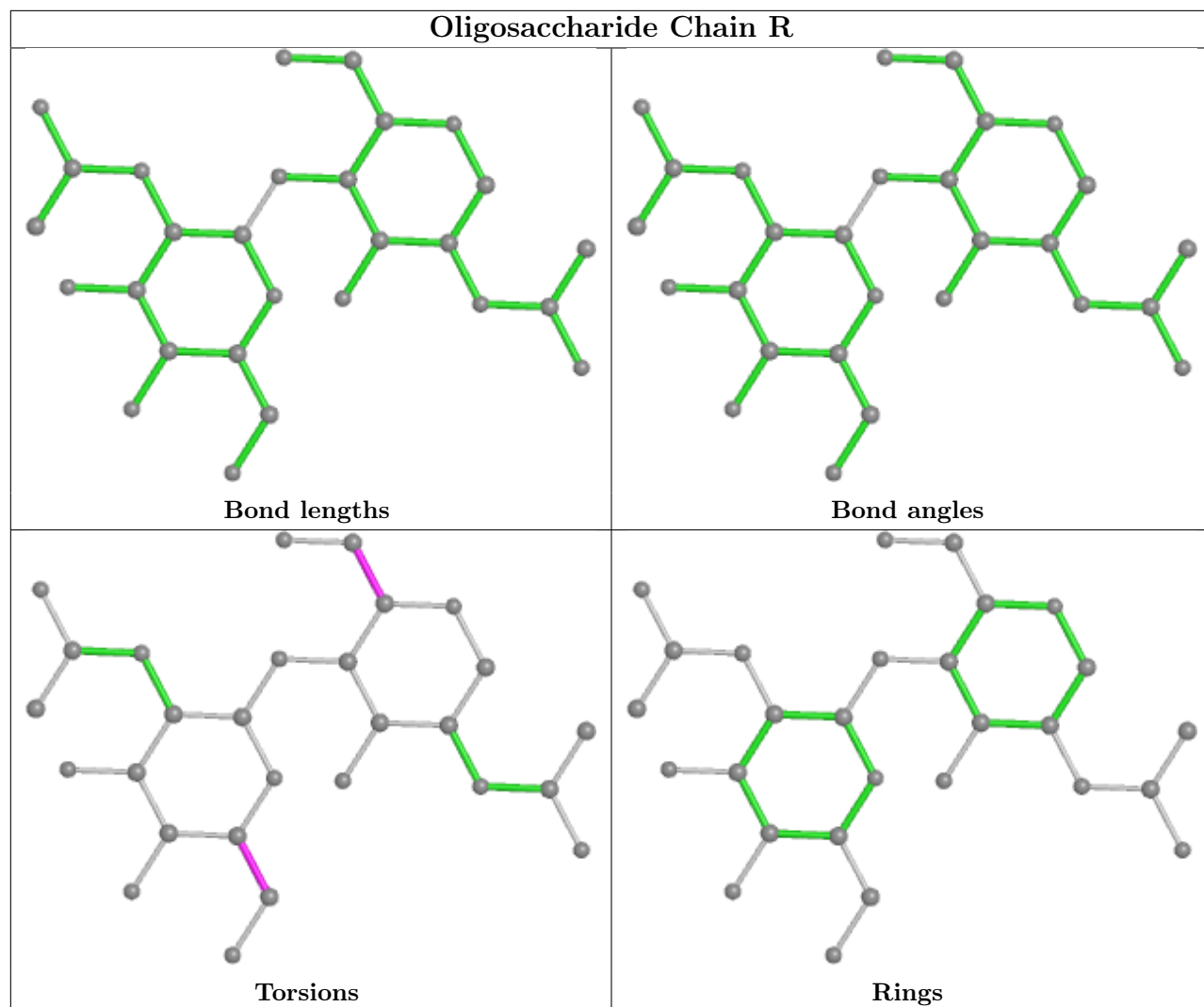


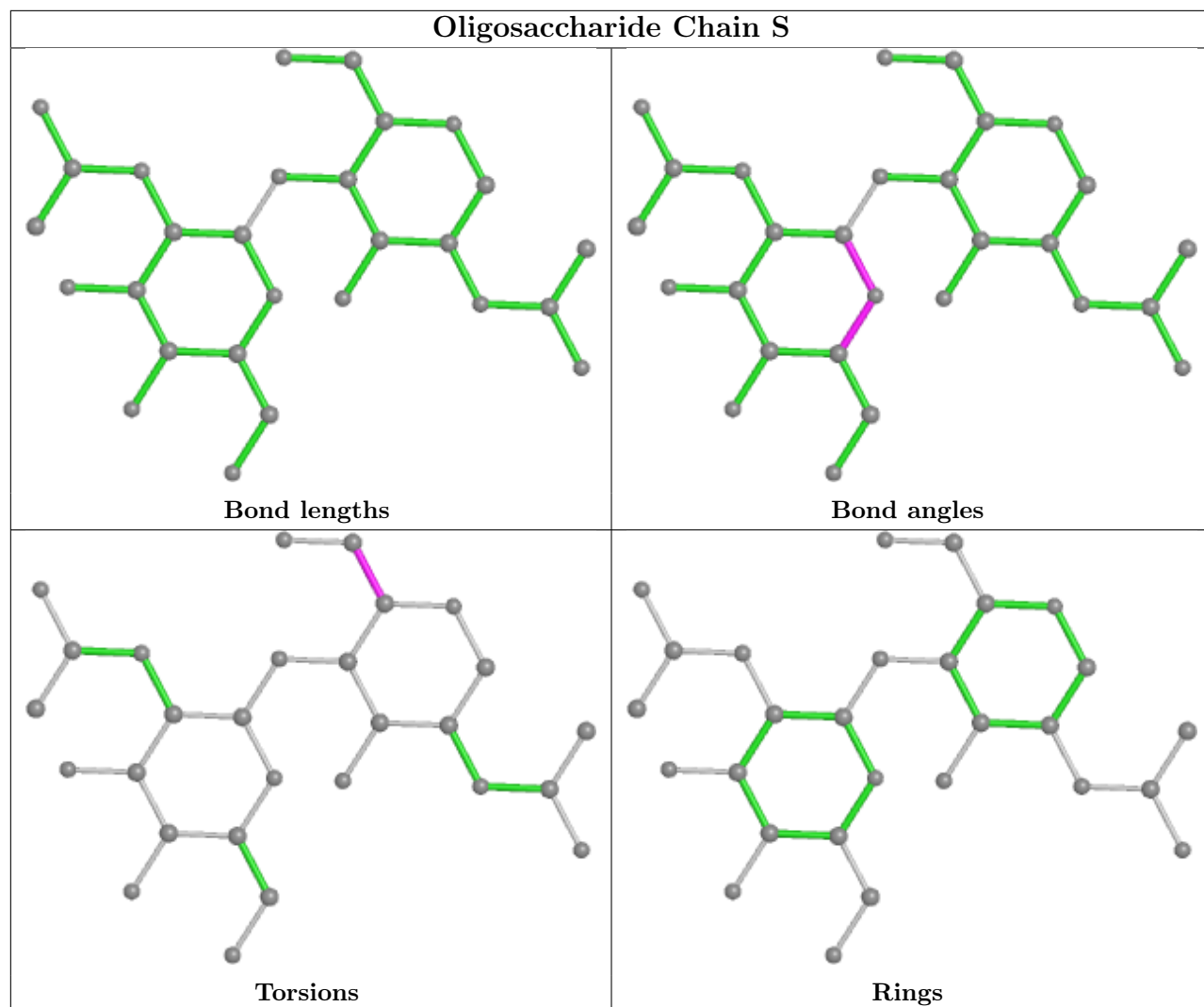


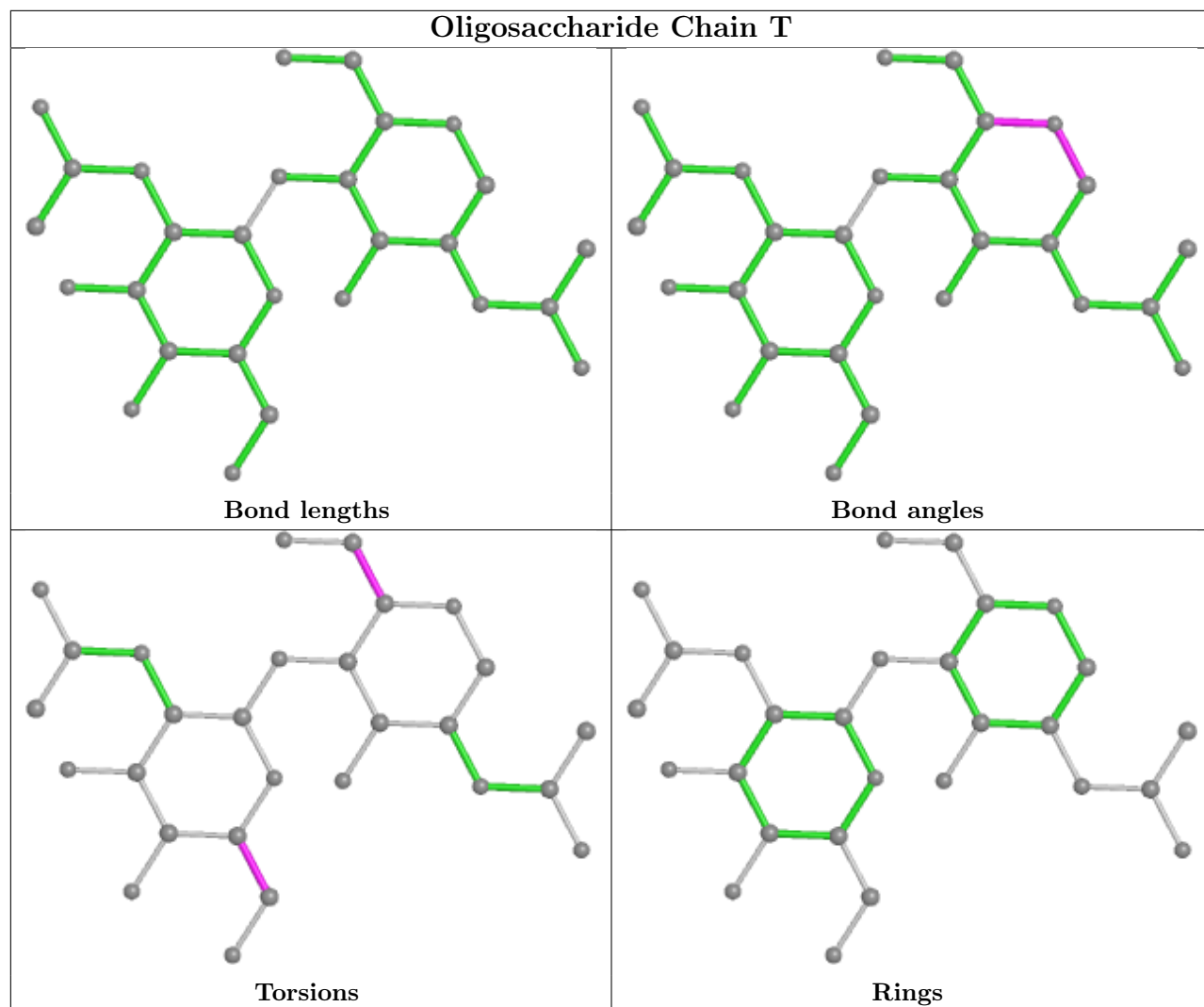


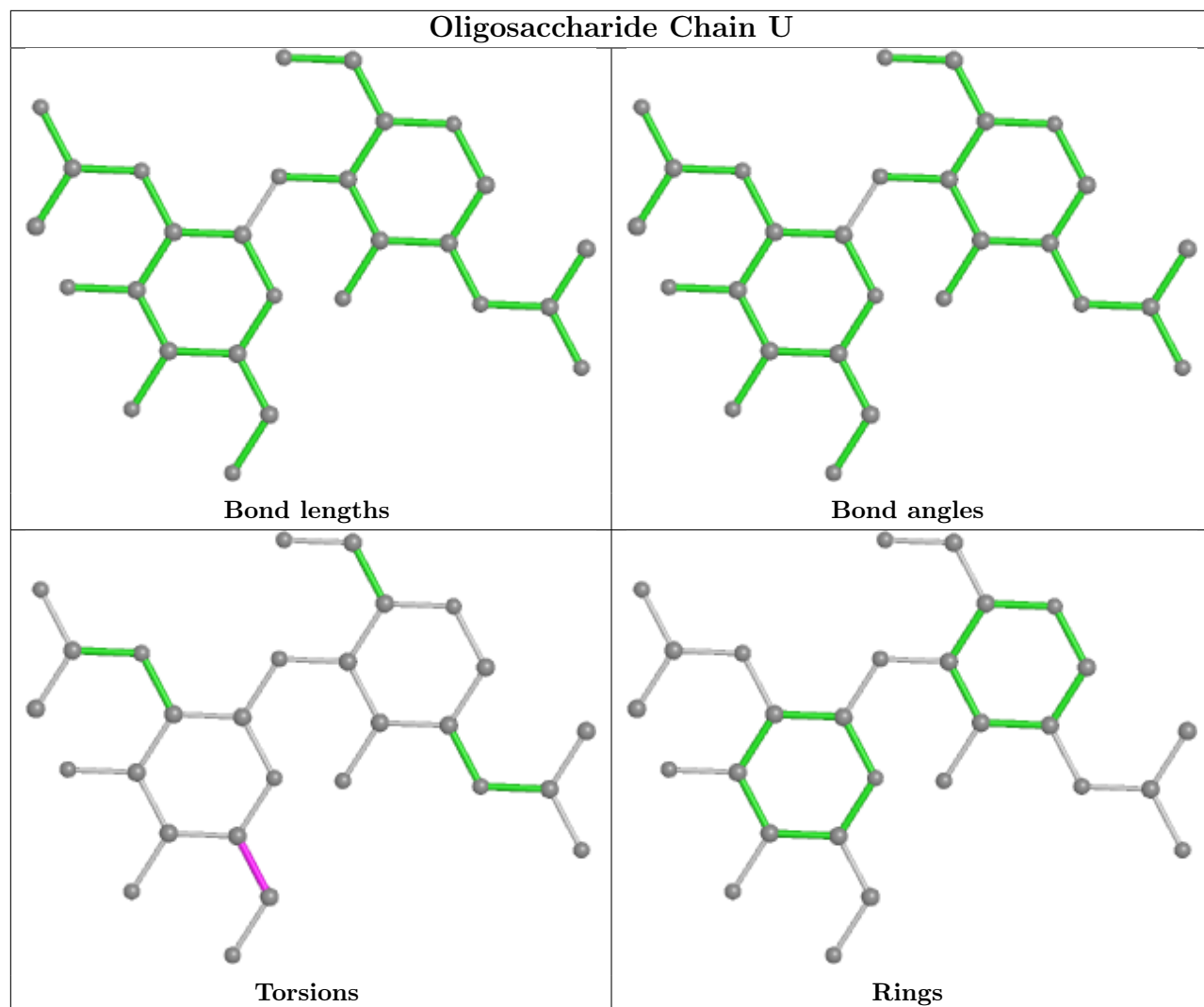


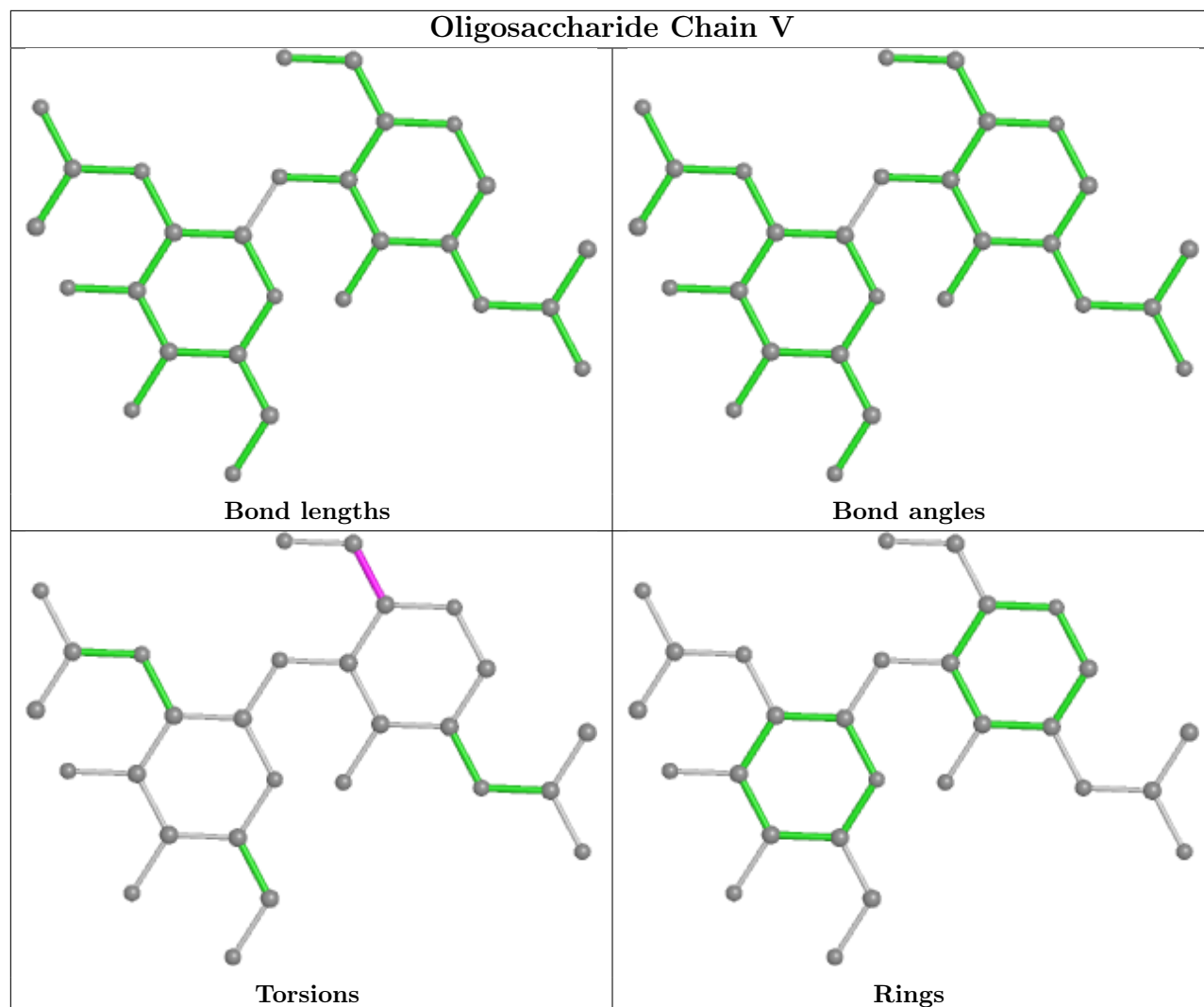


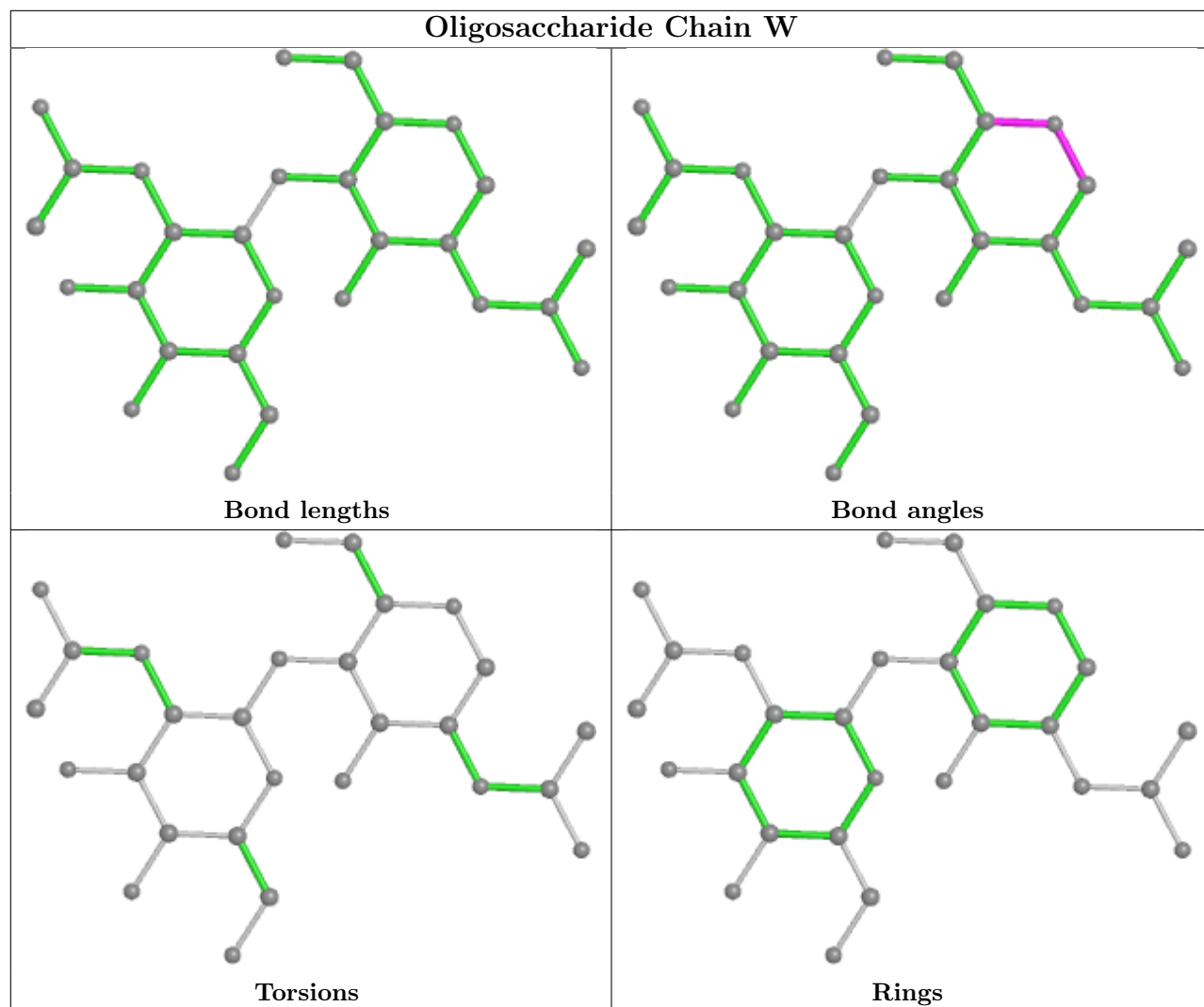


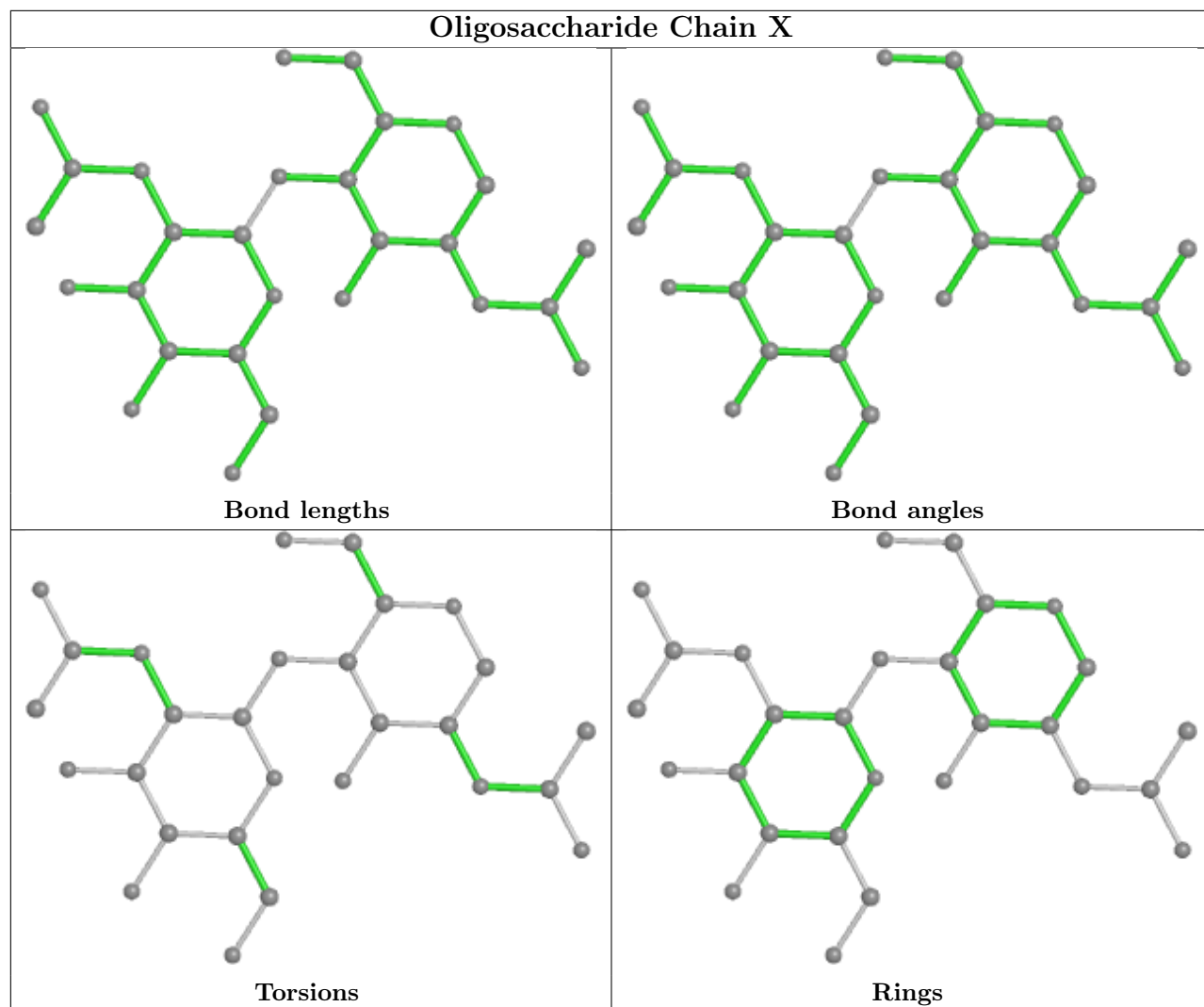


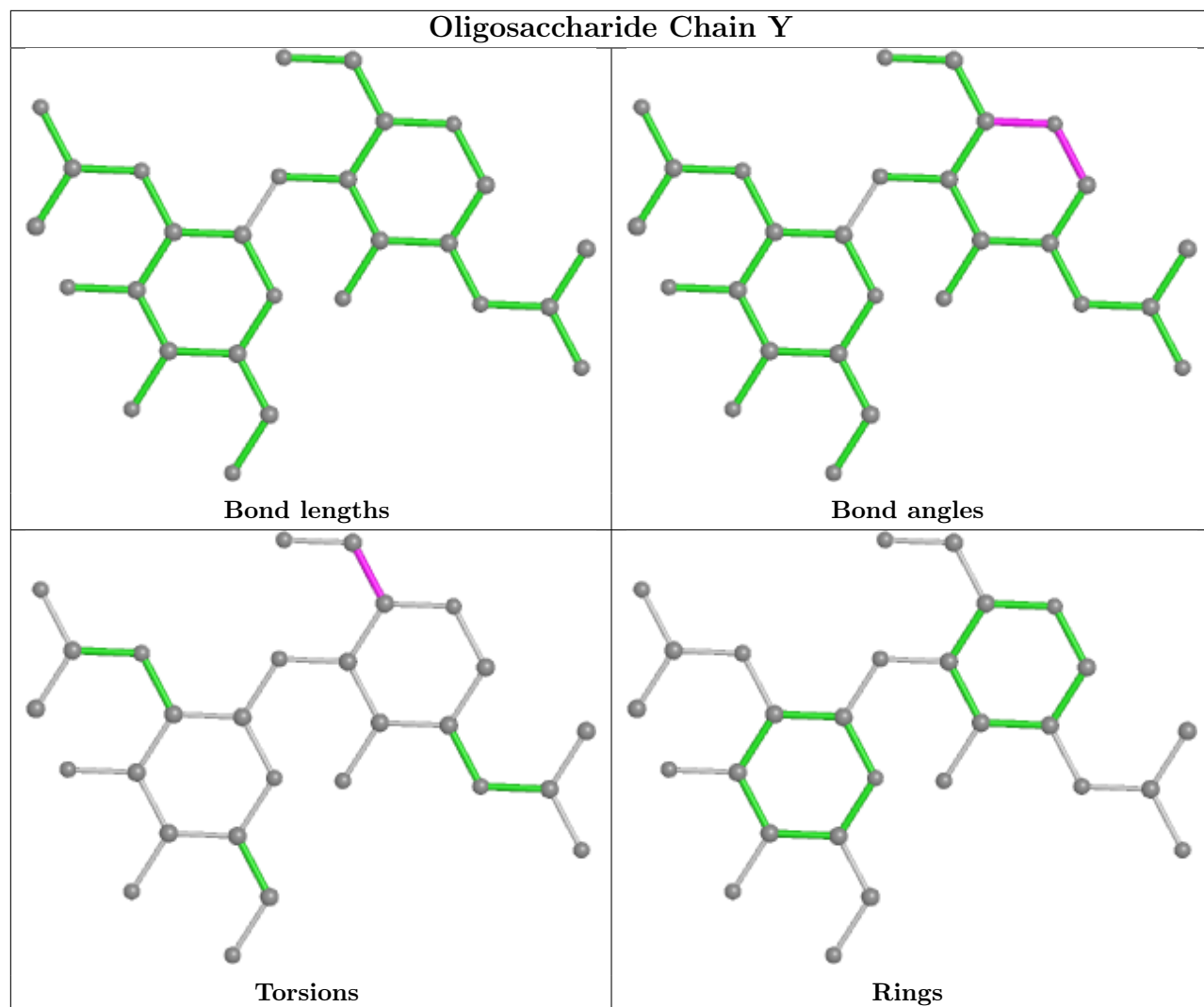


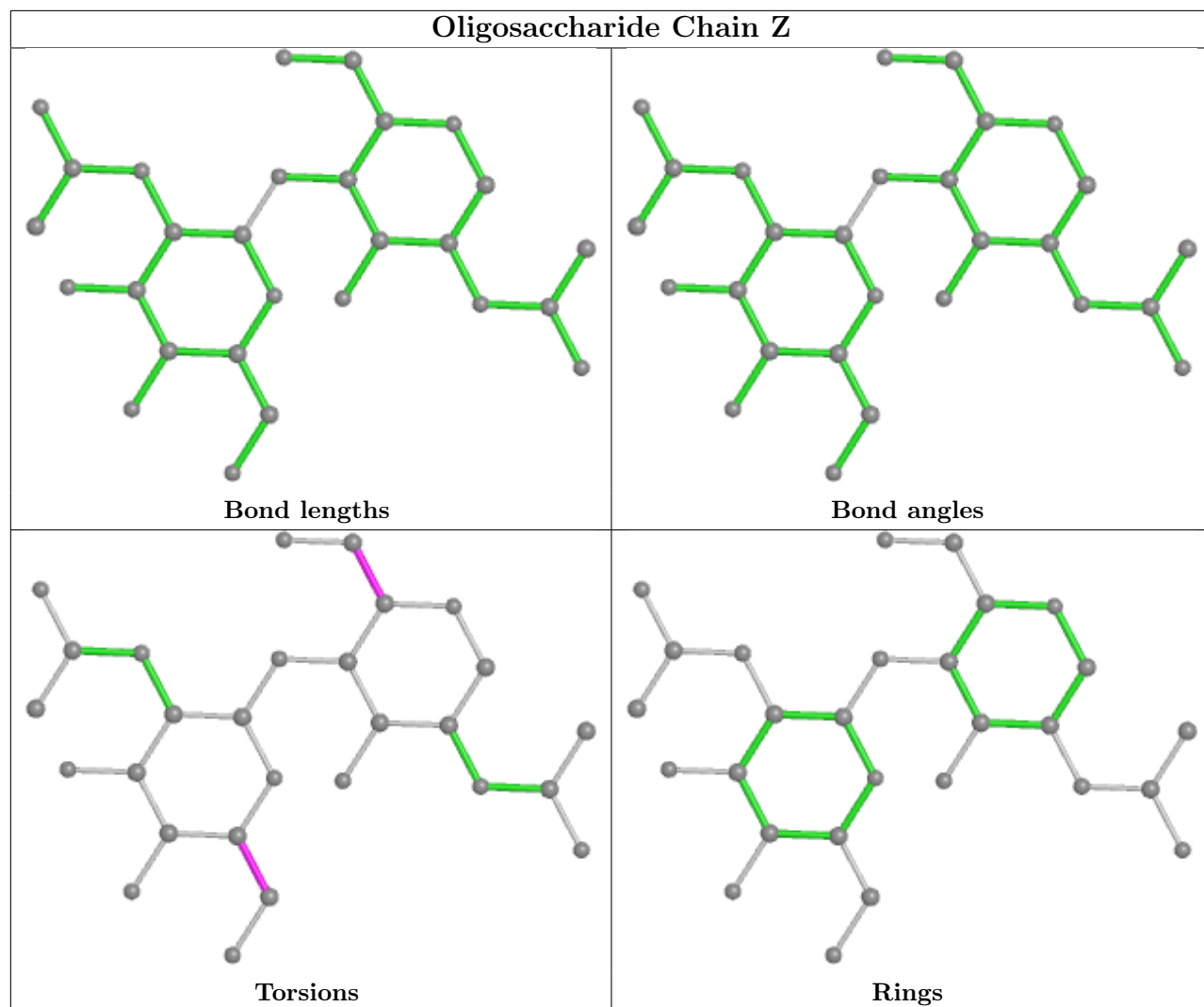


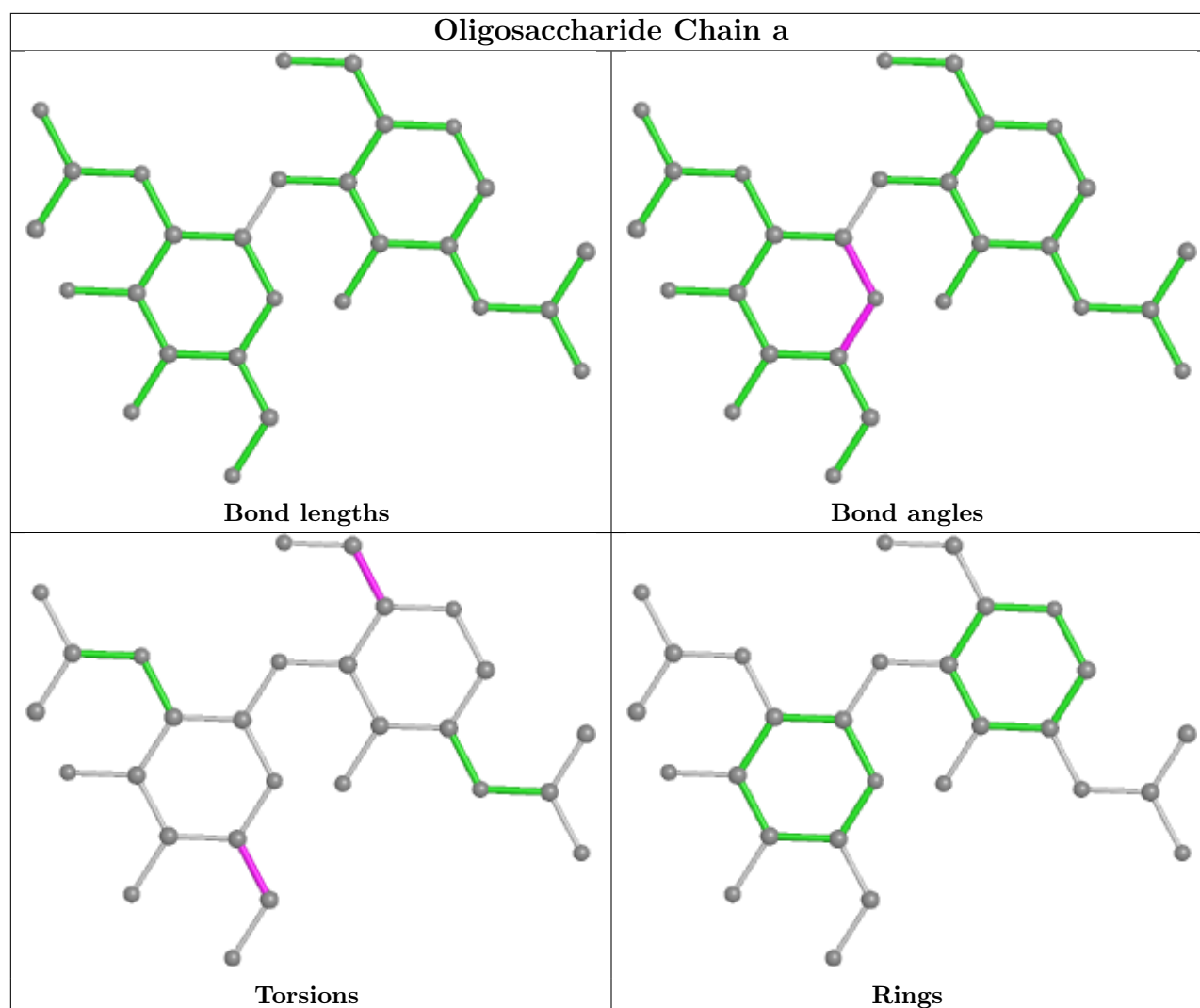












5.6 Ligand geometry [i](#)

39 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	2005	1	14,14,15	0.40	0	17,19,21	0.49	0
4	NAG	A	3003	1	14,14,15	0.58	0	17,19,21	0.51	0
3	PLM	C	2002	-	17,17,17	0.50	0	17,17,17	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLM	A	3001	-	17,17,17	0.59	1 (5%)	17,17,17	1.07	2 (11%)
4	NAG	B	2004	1	14,14,15	0.55	0	17,19,21	0.52	0
4	NAG	B	2011	1	14,14,15	0.37	0	17,19,21	0.61	1 (5%)
4	NAG	A	3006	1	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	C	2004	1	14,14,15	0.42	0	17,19,21	0.52	0
5	OLA	A	3013	-	19,19,19	0.44	0	19,19,19	1.02	1 (5%)
4	NAG	C	2011	1	14,14,15	0.40	0	17,19,21	0.70	1 (5%)
4	NAG	C	2007	1	14,14,15	0.34	0	17,19,21	0.72	1 (5%)
4	NAG	A	3007	1	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	A	3008	1	14,14,15	0.34	0	17,19,21	0.42	0
4	NAG	A	3004	1	14,14,15	0.32	0	17,19,21	0.51	0
4	NAG	B	2012	1	14,14,15	0.33	0	17,19,21	0.54	0
4	NAG	C	2006	1	14,14,15	0.34	0	17,19,21	0.45	0
4	NAG	B	2013	1	14,14,15	0.38	0	17,19,21	0.63	1 (5%)
4	NAG	B	2008	1	14,14,15	0.28	0	17,19,21	0.47	0
4	NAG	B	2006	1	14,14,15	0.45	0	17,19,21	0.50	0
4	NAG	B	2005	1	14,14,15	0.54	0	17,19,21	0.52	0
3	PLM	B	2002	-	17,17,17	0.50	0	17,17,17	0.88	0
4	NAG	A	3010	1	14,14,15	0.30	0	17,19,21	0.72	1 (5%)
4	NAG	C	2008	1	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
4	NAG	A	3009	1	14,14,15	0.48	0	17,19,21	0.56	0
4	NAG	A	3002	1	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	B	2007	1	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	A	3011	1	14,14,15	0.48	0	17,19,21	0.55	0
4	NAG	A	3012	1	14,14,15	0.54	0	17,19,21	0.51	0
5	OLA	C	2001	-	19,19,19	0.40	0	19,19,19	0.95	0
4	NAG	A	3005	1	14,14,15	0.42	0	17,19,21	0.50	0
5	OLA	B	2001	-	19,19,19	0.40	0	19,19,19	1.10	1 (5%)
4	NAG	C	2013	1	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
4	NAG	B	2010	1	14,14,15	0.39	0	17,19,21	0.50	0
4	NAG	B	2003	1	14,14,15	0.37	0	17,19,21	0.63	1 (5%)
4	NAG	C	2012	1	14,14,15	0.46	0	17,19,21	0.64	1 (5%)
4	NAG	C	2010	1	14,14,15	0.30	0	17,19,21	0.44	0
4	NAG	C	2009	1	14,14,15	0.48	0	17,19,21	0.41	0
4	NAG	B	2009	1	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	C	2003	1	14,14,15	0.34	0	17,19,21	0.69	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
4	NAG	C	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	A	3003	1	-	2/6/23/26	0/1/1/1
3	PLM	C	2002	-	-	9/15/15/15	-
3	PLM	A	3001	-	-	9/15/15/15	-
4	NAG	B	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2011	1	-	2/6/23/26	0/1/1/1
4	NAG	A	3006	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
5	OLA	A	3013	-	-	11/17/17/17	-
4	NAG	C	2011	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	A	3007	1	-	1/6/23/26	0/1/1/1
4	NAG	A	3008	1	-	0/6/23/26	0/1/1/1
4	NAG	A	3004	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2012	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2013	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2008	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2005	1	-	2/6/23/26	0/1/1/1
3	PLM	B	2002	-	-	9/15/15/15	-
4	NAG	A	3010	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2008	1	-	0/6/23/26	0/1/1/1
4	NAG	A	3009	1	-	2/6/23/26	0/1/1/1
4	NAG	A	3002	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	A	3011	1	-	2/6/23/26	0/1/1/1
4	NAG	A	3012	1	-	1/6/23/26	0/1/1/1
5	OLA	C	2001	-	-	10/17/17/17	-
4	NAG	A	3005	1	-	1/6/23/26	0/1/1/1
5	OLA	B	2001	-	-	12/17/17/17	-
4	NAG	C	2013	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2010	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2012	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2010	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3001	PLM	O1-C1	-2.17	1.23	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3001	PLM	O1-C1-O2	-2.72	116.51	123.30
5	B	2001	OLA	C3-C2-C1	-2.68	107.73	114.47
4	C	2007	NAG	C1-O5-C5	2.67	115.81	112.19
4	A	3010	NAG	C1-O5-C5	2.57	115.68	112.19
5	A	3013	OLA	C3-C2-C1	-2.53	108.08	114.47
4	C	2003	NAG	C1-O5-C5	2.49	115.56	112.19
4	C	2011	NAG	C1-O5-C5	2.46	115.53	112.19
4	C	2008	NAG	C8-C7-N2	2.31	120.00	116.10
4	C	2013	NAG	C1-O5-C5	2.25	115.24	112.19
4	B	2003	NAG	C1-O5-C5	2.20	115.18	112.19
3	A	3001	PLM	O1-C1-C2	2.19	121.08	114.03
4	C	2012	NAG	C1-O5-C5	2.18	115.15	112.19
4	B	2013	NAG	C1-O5-C5	2.15	115.11	112.19
4	B	2011	NAG	C1-O5-C5	2.12	115.07	112.19

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3003	NAG	O5-C5-C6-O6
4	B	2004	NAG	O5-C5-C6-O6
4	B	2005	NAG	O5-C5-C6-O6
4	A	3002	NAG	O5-C5-C6-O6
4	A	3010	NAG	O5-C5-C6-O6
4	B	2003	NAG	O5-C5-C6-O6
4	B	2007	NAG	O5-C5-C6-O6
4	B	2011	NAG	O5-C5-C6-O6
4	C	2007	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	2011	NAG	O5-C5-C6-O6
4	A	3011	NAG	O5-C5-C6-O6
4	B	2010	NAG	O5-C5-C6-O6
4	C	2010	NAG	O5-C5-C6-O6
4	C	2013	NAG	O5-C5-C6-O6
4	B	2007	NAG	C4-C5-C6-O6
4	B	2013	NAG	C4-C5-C6-O6
4	B	2003	NAG	C4-C5-C6-O6
4	B	2011	NAG	C4-C5-C6-O6
4	C	2007	NAG	C4-C5-C6-O6
4	B	2013	NAG	O5-C5-C6-O6
4	A	3002	NAG	C4-C5-C6-O6
4	C	2011	NAG	C4-C5-C6-O6
4	C	2006	NAG	O5-C5-C6-O6
4	A	3003	NAG	C4-C5-C6-O6
4	B	2005	NAG	C4-C5-C6-O6
4	C	2012	NAG	C4-C5-C6-O6
4	A	3009	NAG	O5-C5-C6-O6
4	A	3010	NAG	C4-C5-C6-O6
4	B	2004	NAG	C4-C5-C6-O6
4	C	2003	NAG	C4-C5-C6-O6
4	C	2006	NAG	C4-C5-C6-O6
4	C	2010	NAG	C4-C5-C6-O6
4	C	2005	NAG	O5-C5-C6-O6
4	B	2009	NAG	C4-C5-C6-O6
4	B	2010	NAG	C4-C5-C6-O6
4	A	3009	NAG	C4-C5-C6-O6
4	B	2012	NAG	O5-C5-C6-O6
4	C	2005	NAG	C4-C5-C6-O6
4	C	2004	NAG	O5-C5-C6-O6
4	C	2013	NAG	C4-C5-C6-O6
4	C	2003	NAG	O5-C5-C6-O6
4	A	3011	NAG	C4-C5-C6-O6
3	B	2002	PLM	C1-C2-C3-C4
3	C	2002	PLM	C9-CA-CB-CC
5	B	2001	OLA	C2-C3-C4-C5
5	A	3013	OLA	C2-C3-C4-C5
5	A	3013	OLA	C13-C14-C15-C16
5	B	2001	OLA	C5-C6-C7-C8
3	A	3001	PLM	CA-CB-CC-CD
4	C	2012	NAG	O5-C5-C6-O6
5	C	2001	OLA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	C	2001	OLA	C5-C6-C7-C8
3	A	3001	PLM	C2-C3-C4-C5
5	A	3013	OLA	C12-C13-C14-C15
5	C	2001	OLA	C6-C7-C8-C9
5	B	2001	OLA	C1-C2-C3-C4
3	A	3001	PLM	CC-CD-CE-CF
4	B	2009	NAG	O5-C5-C6-O6
3	B	2002	PLM	C8-C9-CA-CB
3	B	2002	PLM	C3-C4-C5-C6
5	A	3013	OLA	C1-C2-C3-C4
3	A	3001	PLM	C9-CA-CB-CC
3	B	2002	PLM	C7-C8-C9-CA
3	A	3001	PLM	C5-C6-C7-C8
5	A	3013	OLA	C6-C7-C8-C9
3	C	2002	PLM	C7-C8-C9-CA
4	A	3012	NAG	O5-C5-C6-O6
3	C	2002	PLM	CC-CD-CE-CF
5	B	2001	OLA	C6-C7-C8-C9
3	A	3001	PLM	C6-C7-C8-C9
5	C	2001	OLA	C3-C4-C5-C6
4	B	2006	NAG	C4-C5-C6-O6
4	C	2009	NAG	C4-C5-C6-O6
3	C	2002	PLM	C2-C3-C4-C5
4	C	2009	NAG	O5-C5-C6-O6
3	A	3001	PLM	C8-C9-CA-CB
3	B	2002	PLM	CC-CD-CE-CF
3	B	2002	PLM	C6-C7-C8-C9
3	B	2002	PLM	CD-CE-CF-CG
4	C	2004	NAG	C4-C5-C6-O6
5	B	2001	OLA	C3-C4-C5-C6
3	C	2002	PLM	CA-CB-CC-CD
5	B	2001	OLA	C15-C16-C17-C18
5	A	3013	OLA	C5-C6-C7-C8
4	A	3007	NAG	C4-C5-C6-O6
3	C	2002	PLM	C1-C2-C3-C4
3	A	3001	PLM	C7-C8-C9-CA
5	B	2001	OLA	C7-C8-C9-C10
3	B	2002	PLM	C2-C3-C4-C5
4	B	2006	NAG	O5-C5-C6-O6
5	B	2001	OLA	C4-C5-C6-C7
4	A	3005	NAG	C4-C5-C6-O6
3	C	2002	PLM	CB-CC-CD-CE

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Mol	Chain	Res	Type	Atoms
5	B	2001	OLA	C13-C14-C15-C16
5	C	2001	OLA	C11-C12-C13-C14
5	C	2001	OLA	C7-C8-C9-C10
5	C	2001	OLA	O2-C1-C2-C3
5	A	3013	OLA	C15-C16-C17-C18
3	C	2002	PLM	CD-CE-CF-CG
5	C	2001	OLA	O1-C1-C2-C3
3	A	3001	PLM	O2-C1-C2-C3
3	C	2002	PLM	C4-C5-C6-C7
5	B	2001	OLA	O2-C1-C2-C3
5	A	3013	OLA	C7-C8-C9-C10
5	A	3013	OLA	C11-C12-C13-C14
3	B	2002	PLM	C9-CA-CB-CC
5	B	2001	OLA	O1-C1-C2-C3
5	A	3013	OLA	O2-C1-C2-C3
5	B	2001	OLA	C11-C12-C13-C14
5	C	2001	OLA	C12-C13-C14-C15
5	A	3013	OLA	O1-C1-C2-C3
5	C	2001	OLA	C13-C14-C15-C16

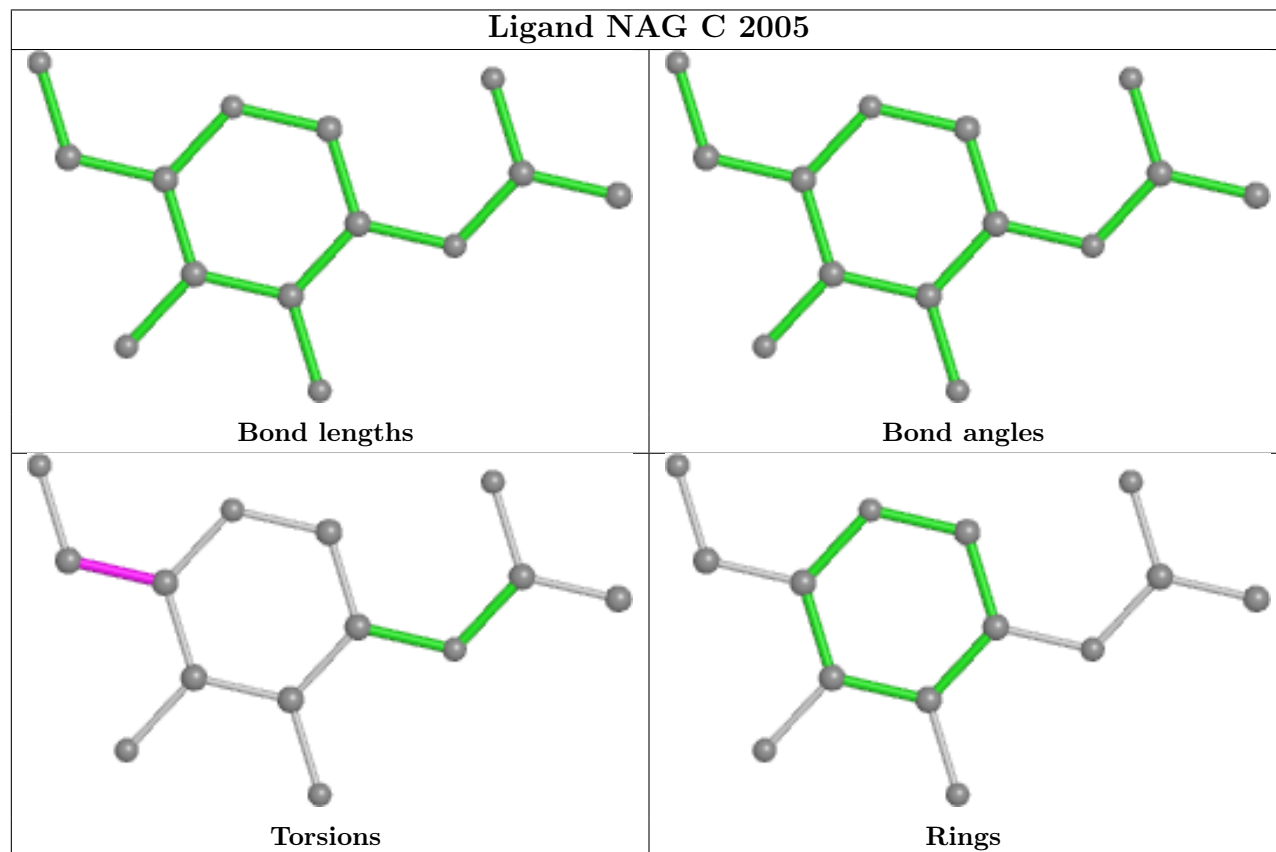
There are no ring outliers.

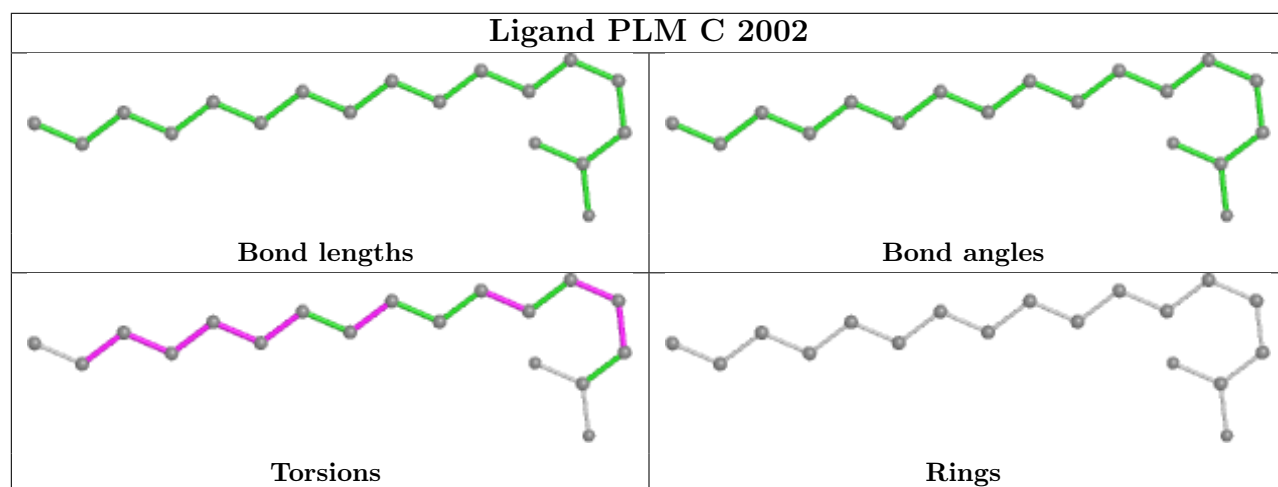
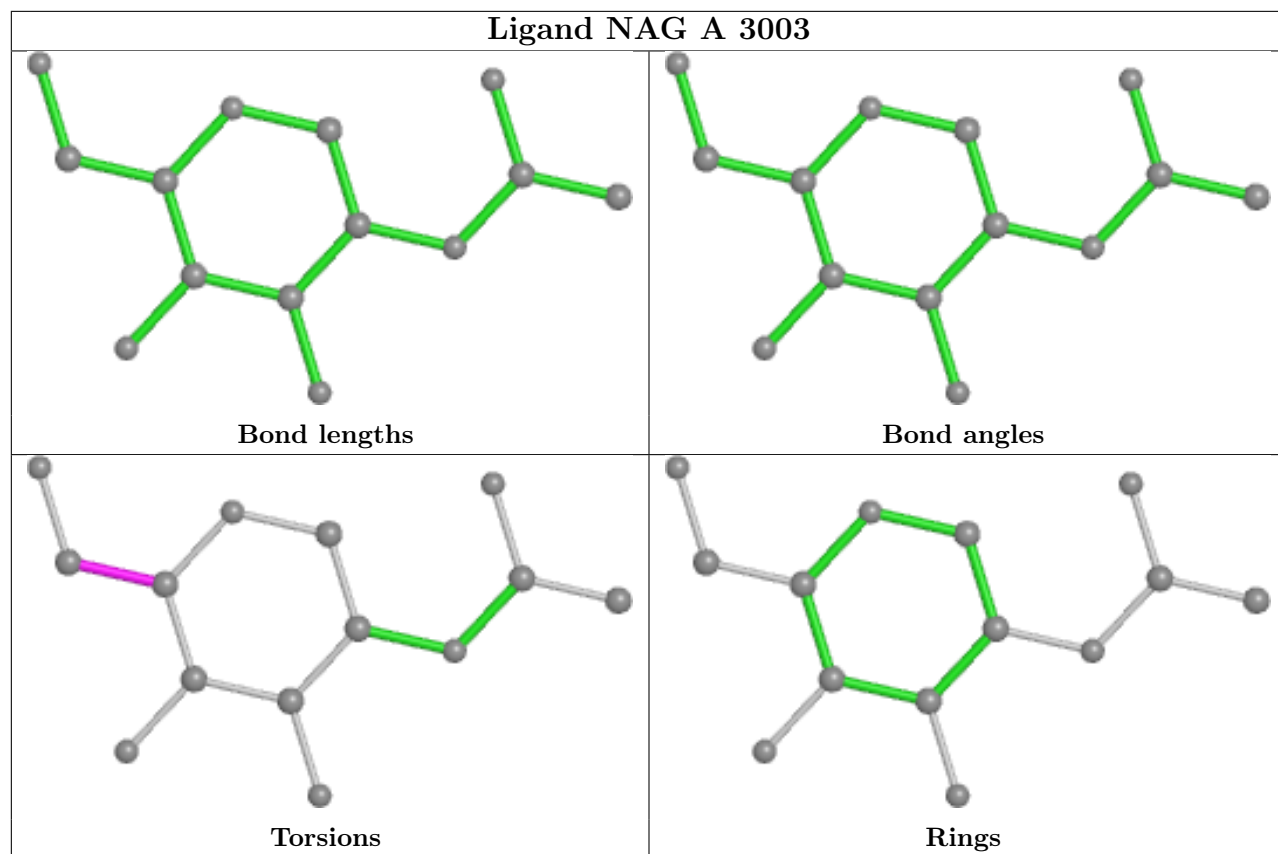
11 monomers are involved in 66 short contacts:

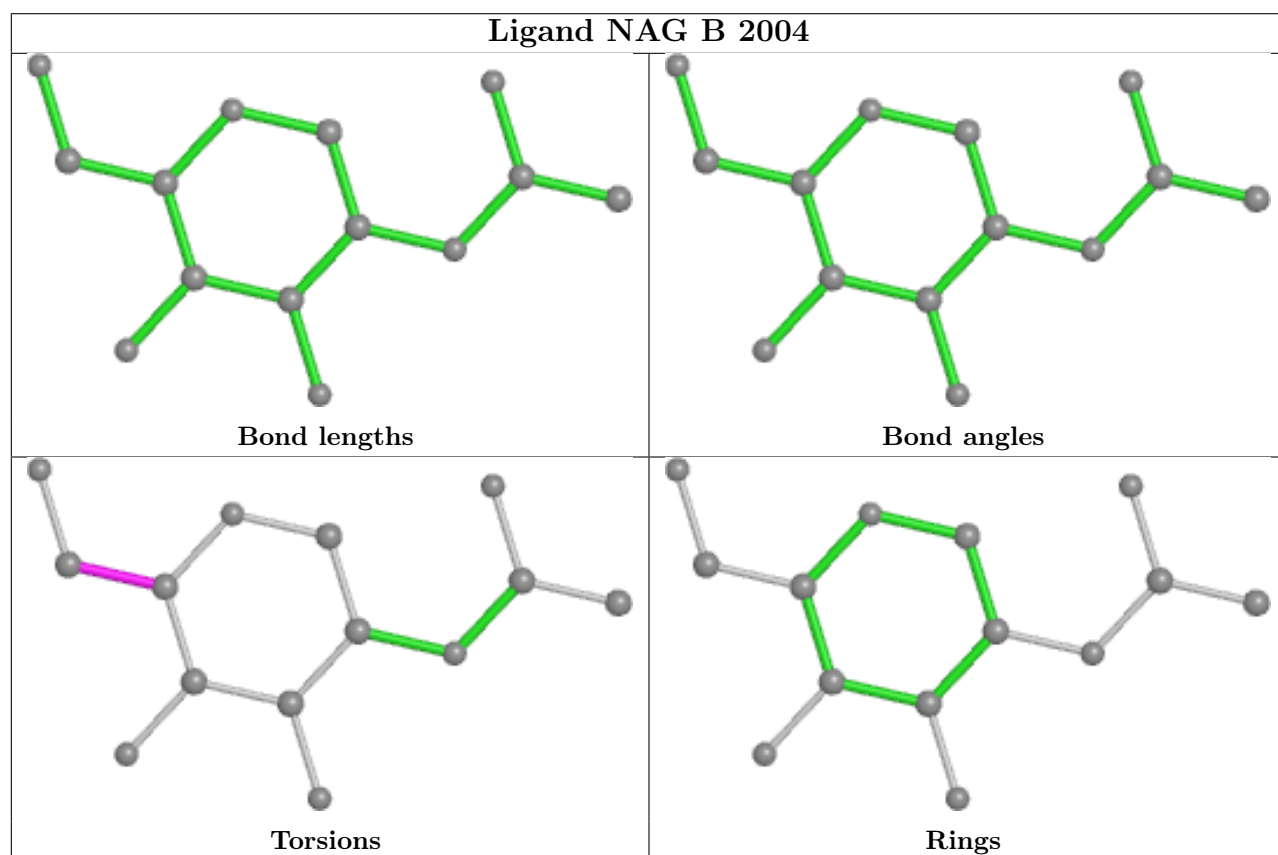
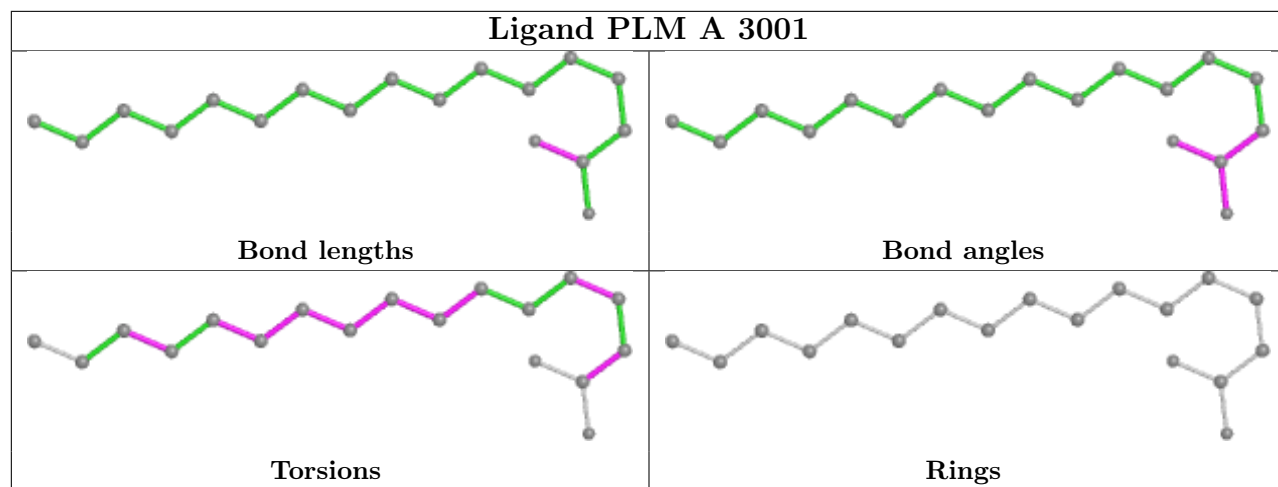
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2002	PLM	16	0
3	A	3001	PLM	15	0
5	A	3013	OLA	1	0
4	A	3007	NAG	4	0
4	B	2008	NAG	2	0
3	B	2002	PLM	23	0
4	A	3002	NAG	1	0
5	C	2001	OLA	1	0
5	B	2001	OLA	1	0
4	B	2003	NAG	1	0
4	C	2003	NAG	1	0

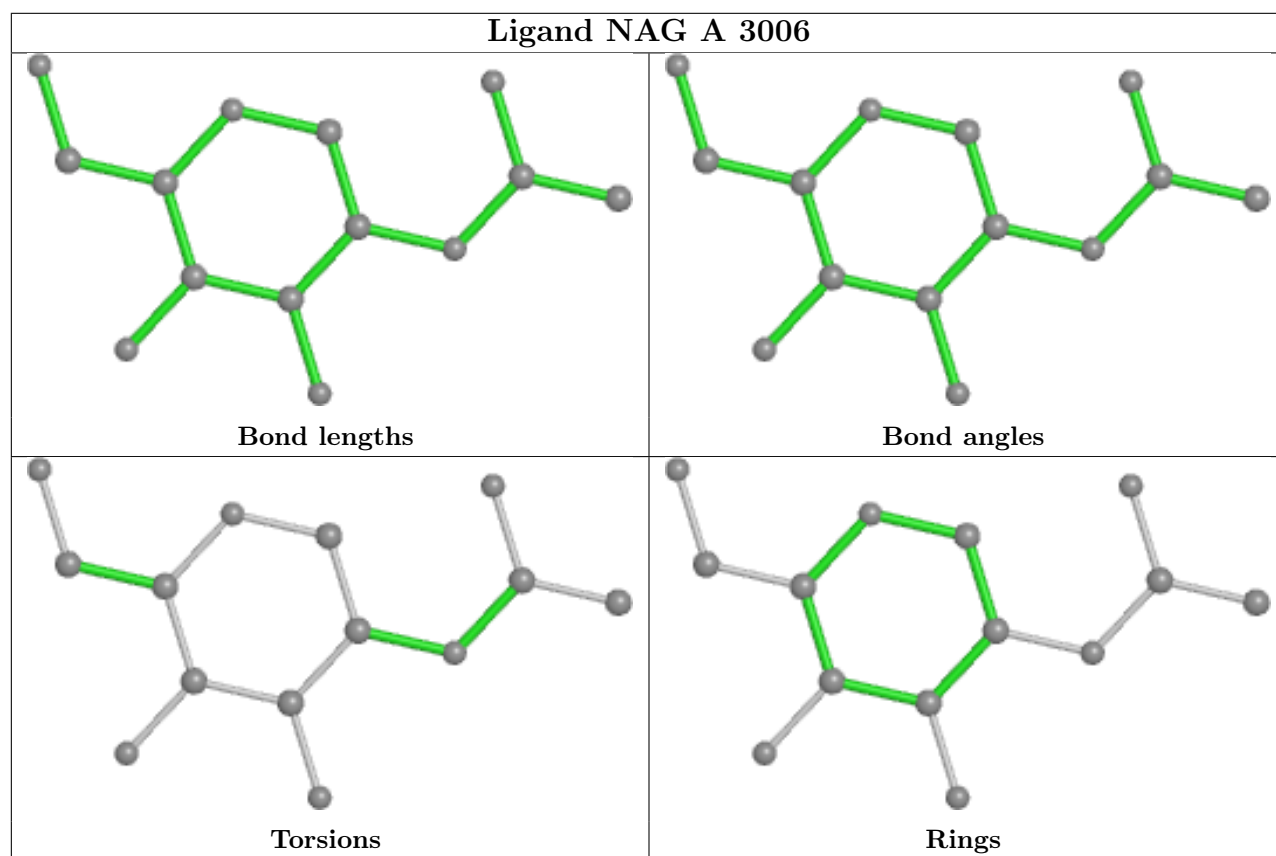
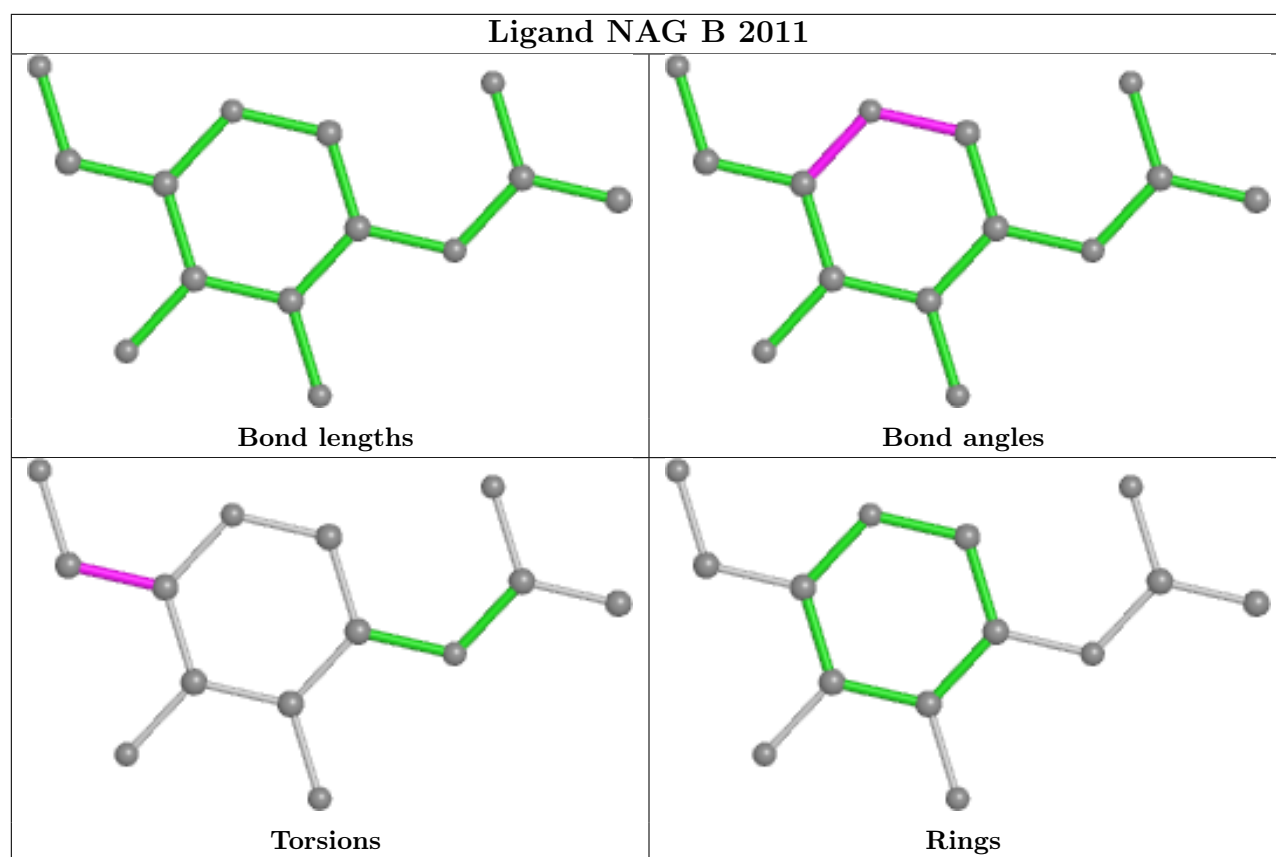
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

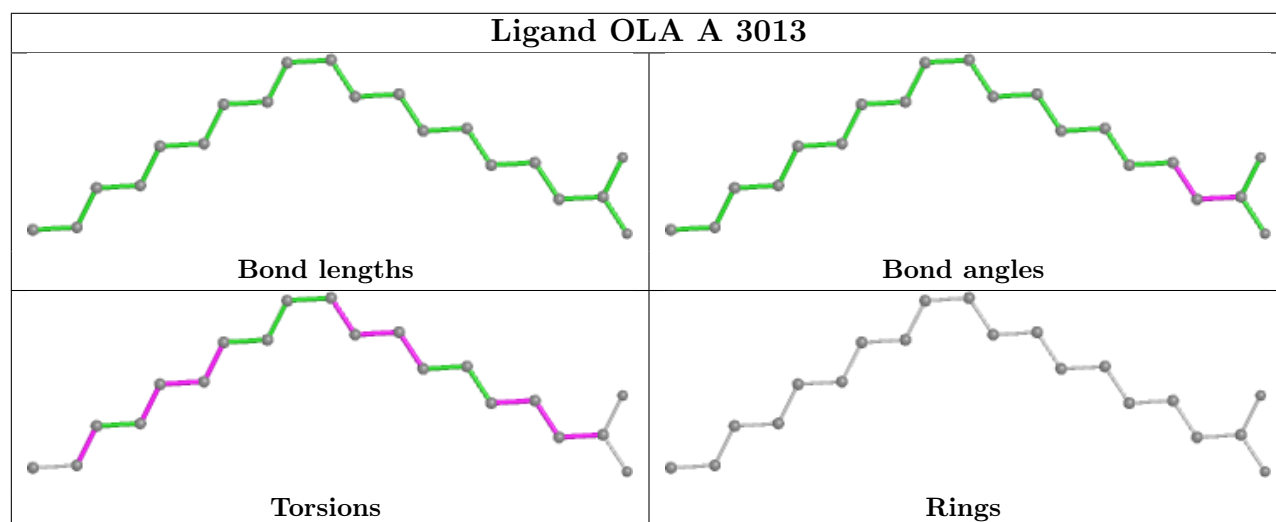
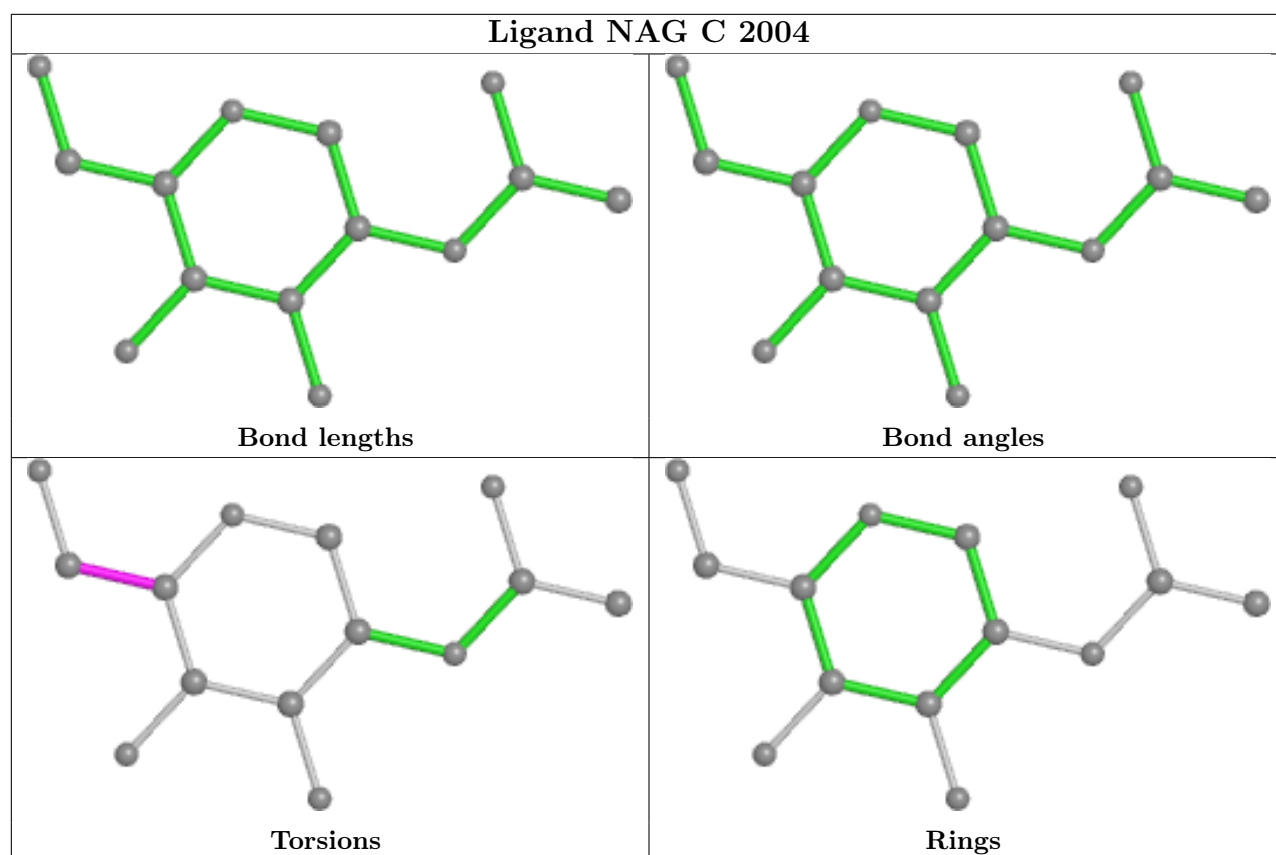
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

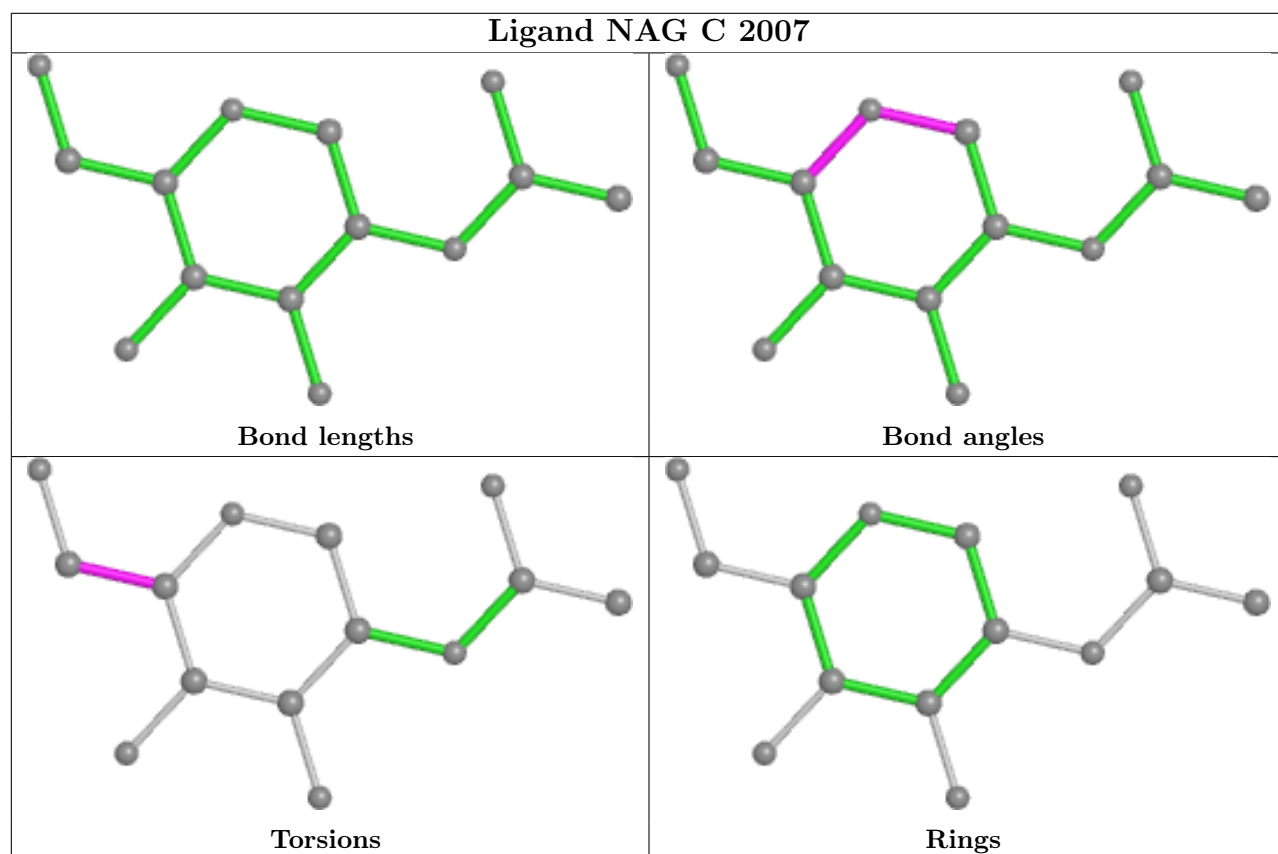
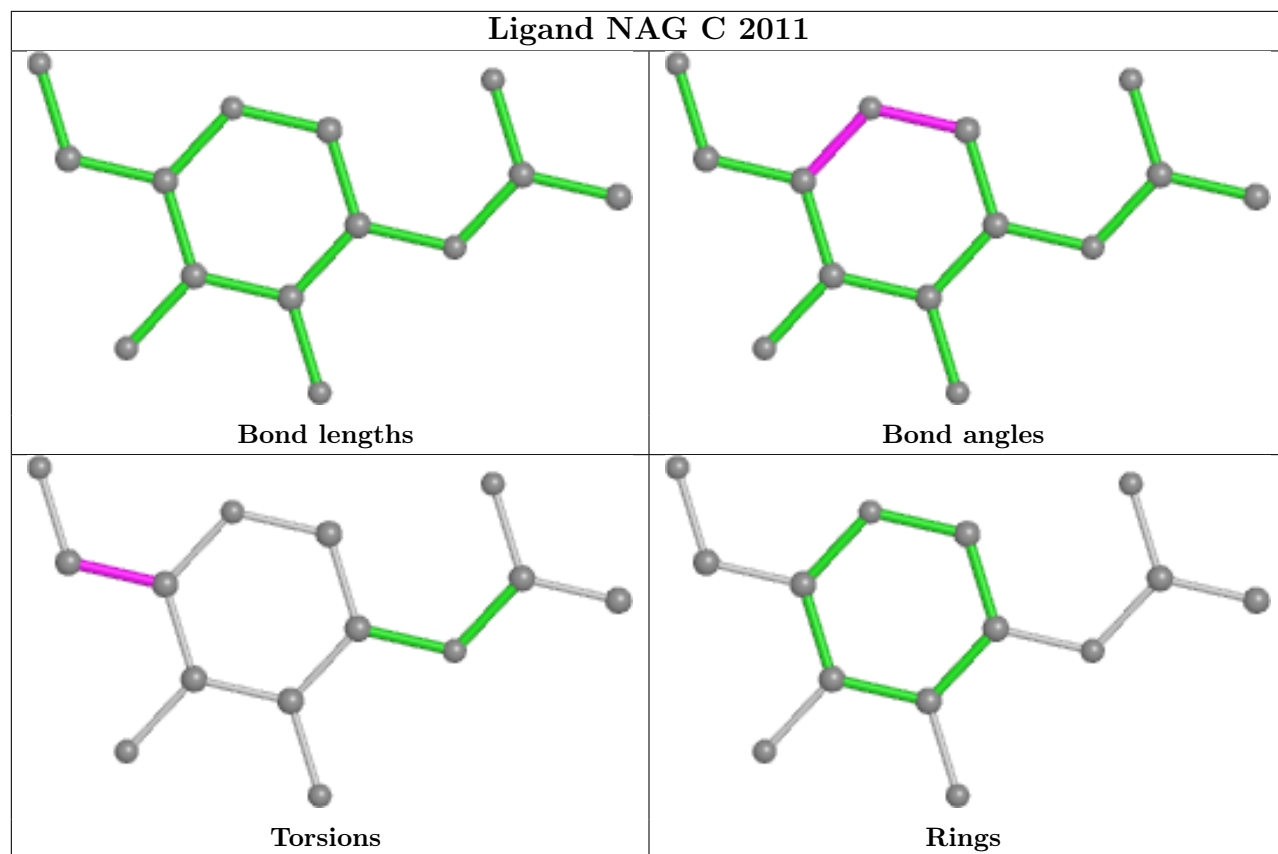




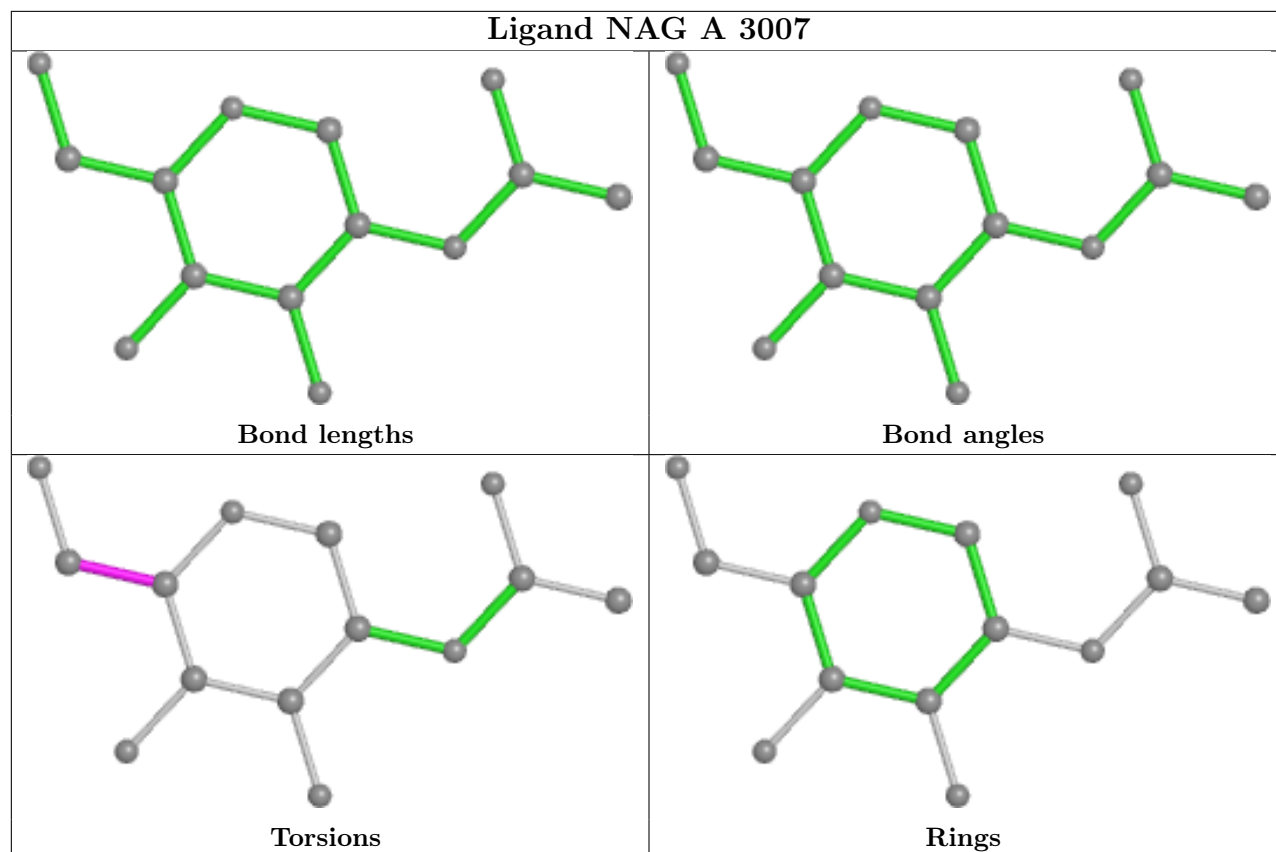




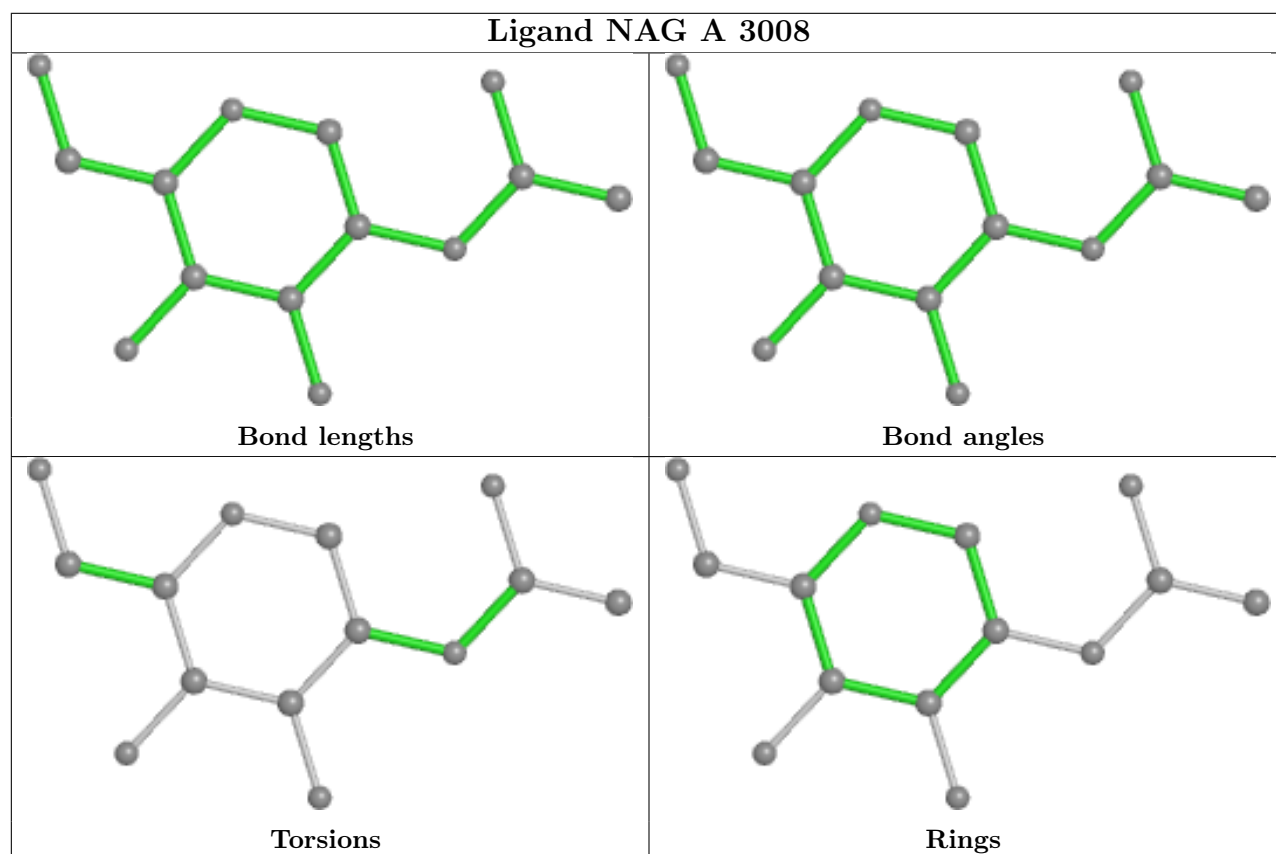


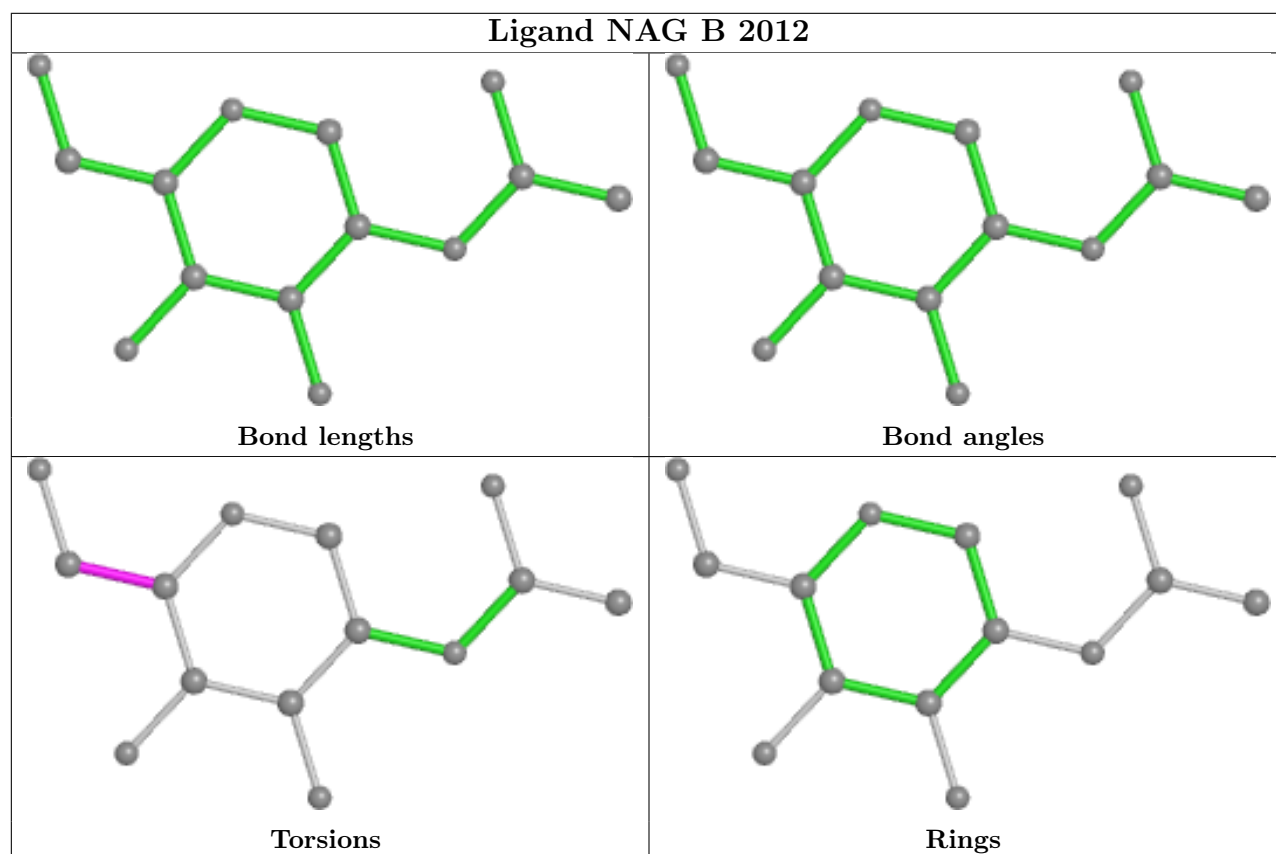
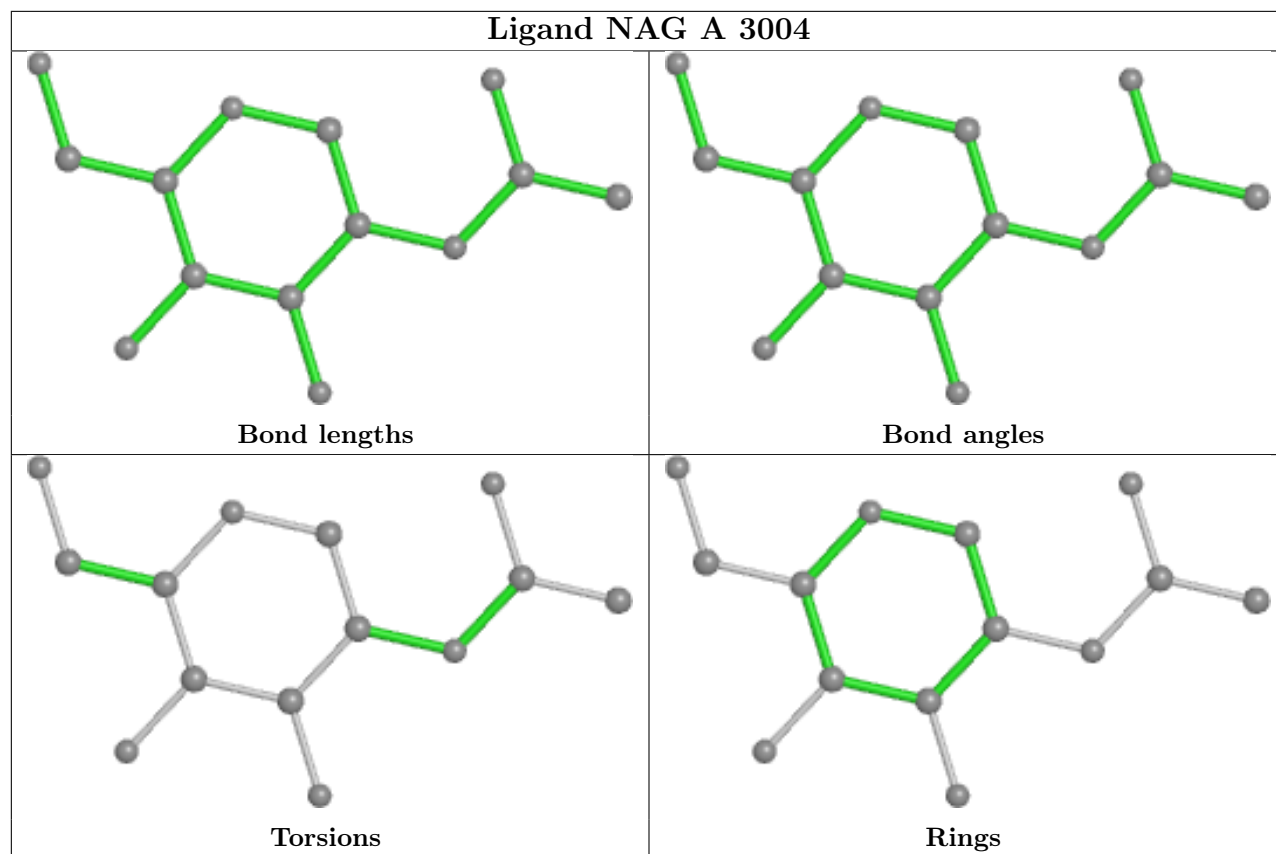


Ligand NAG A 3007

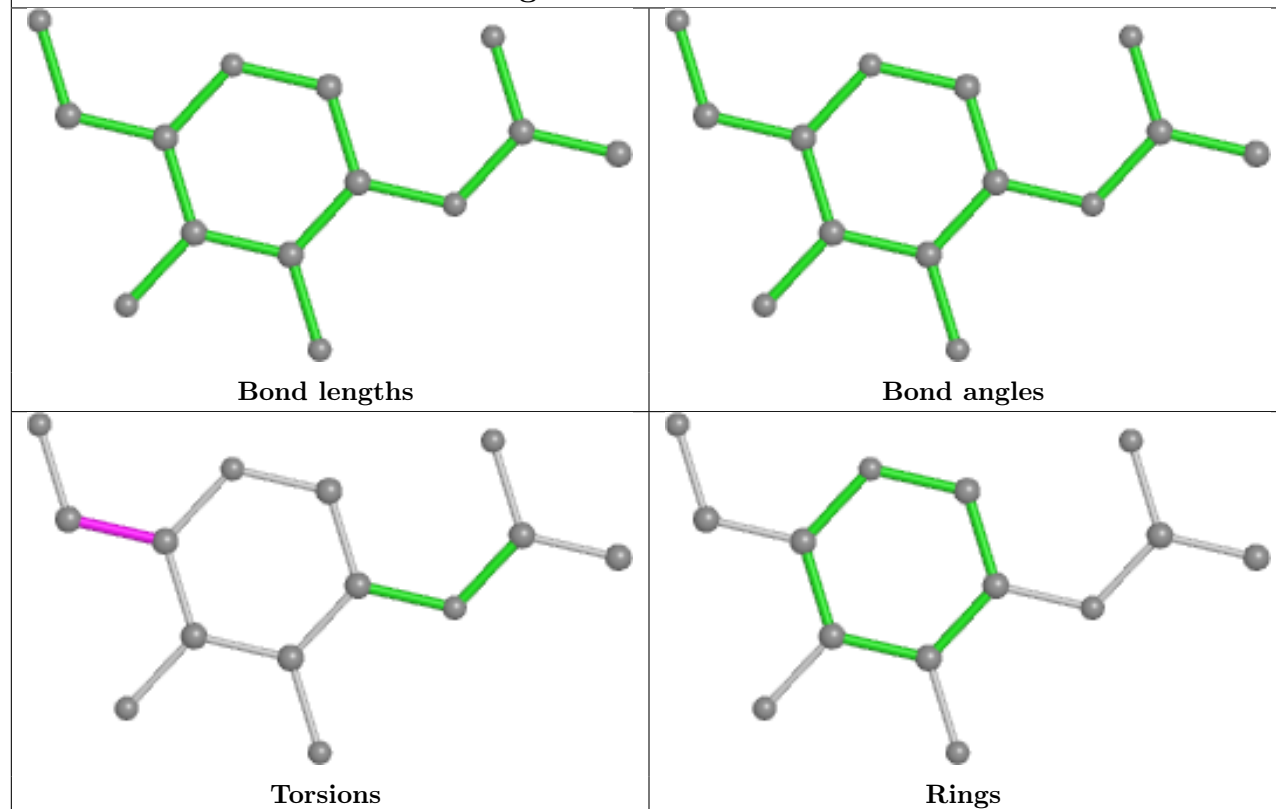


Ligand NAG A 3008

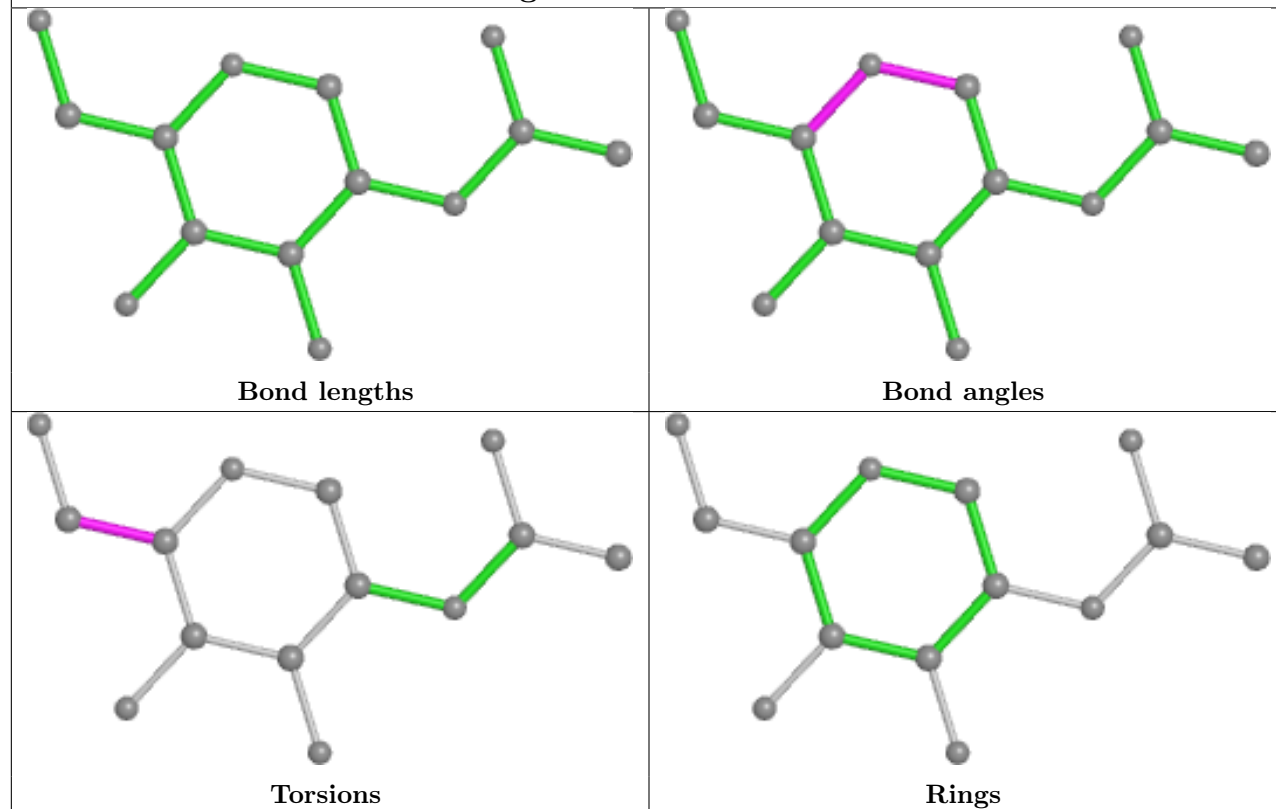


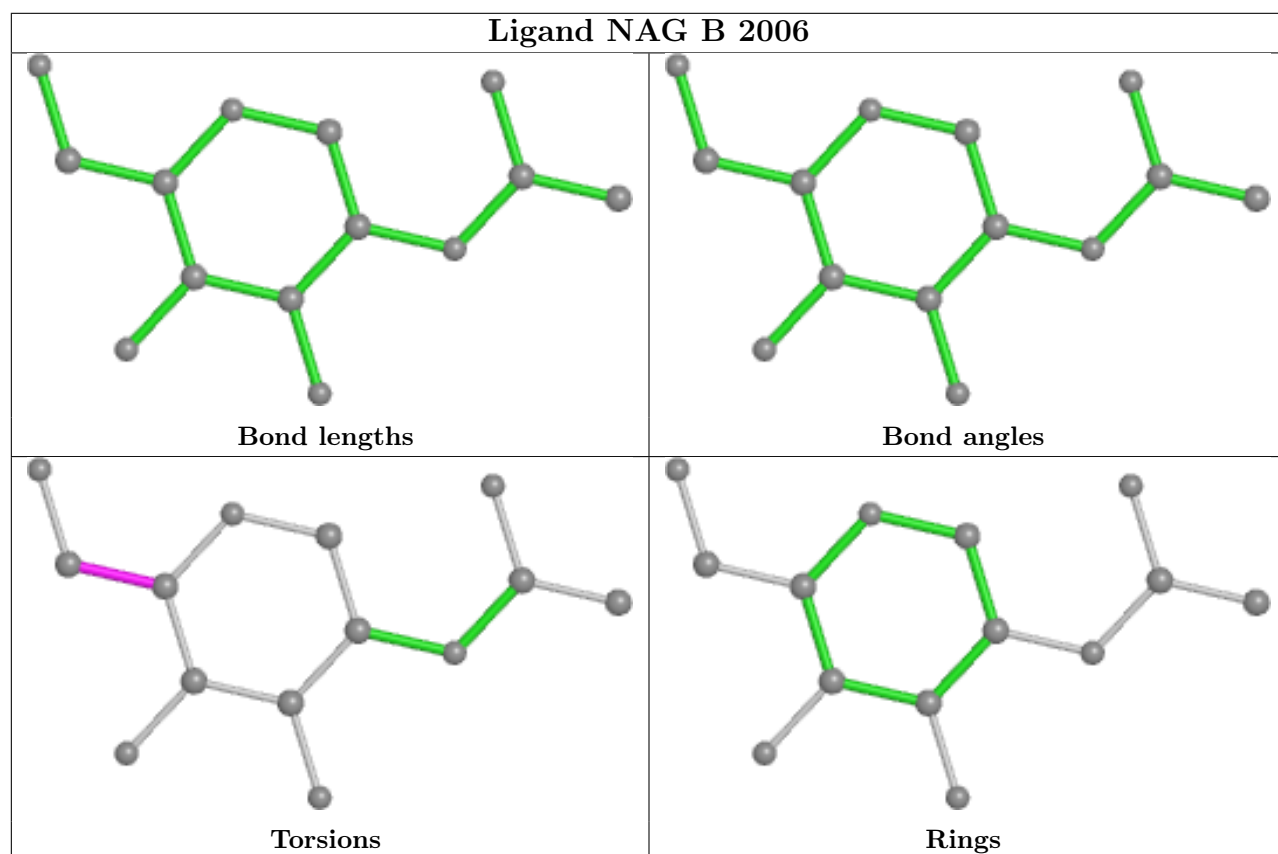
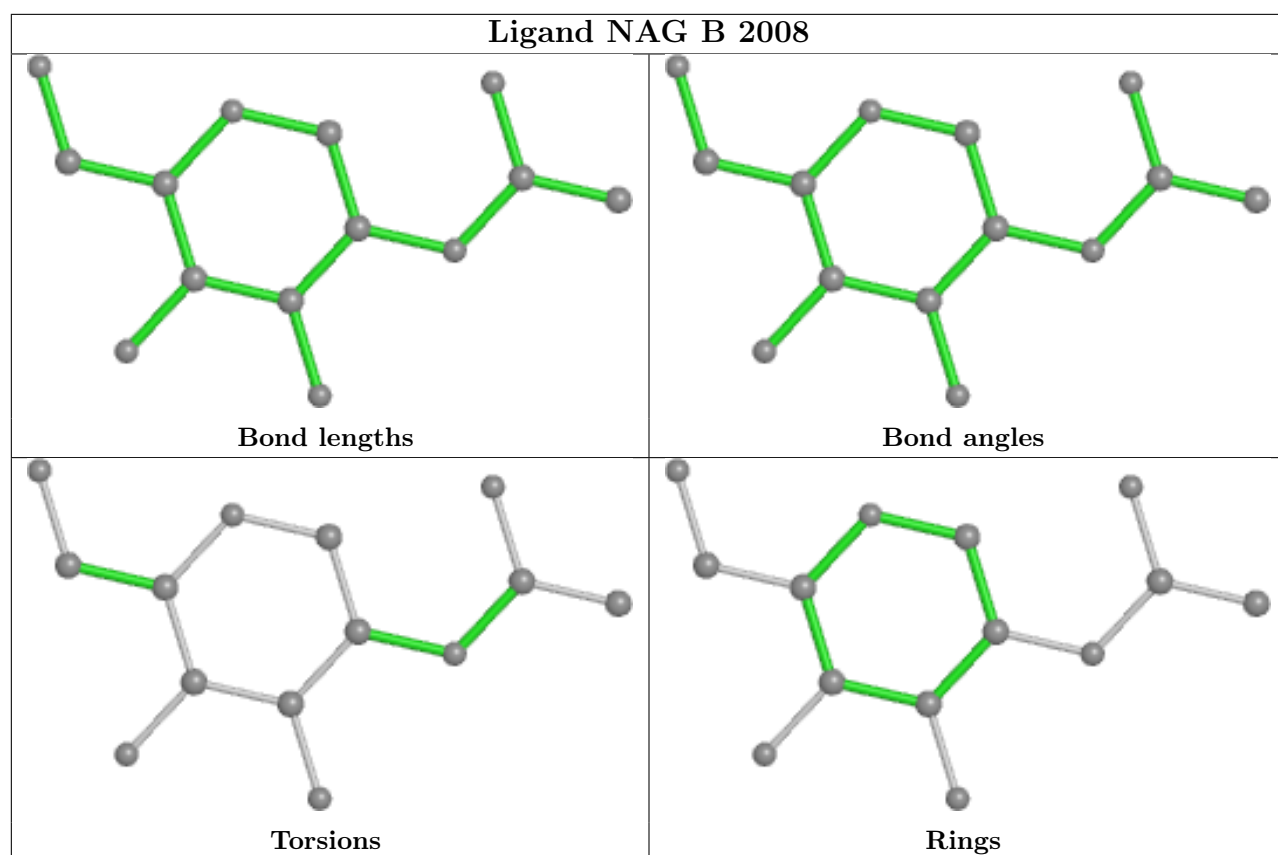


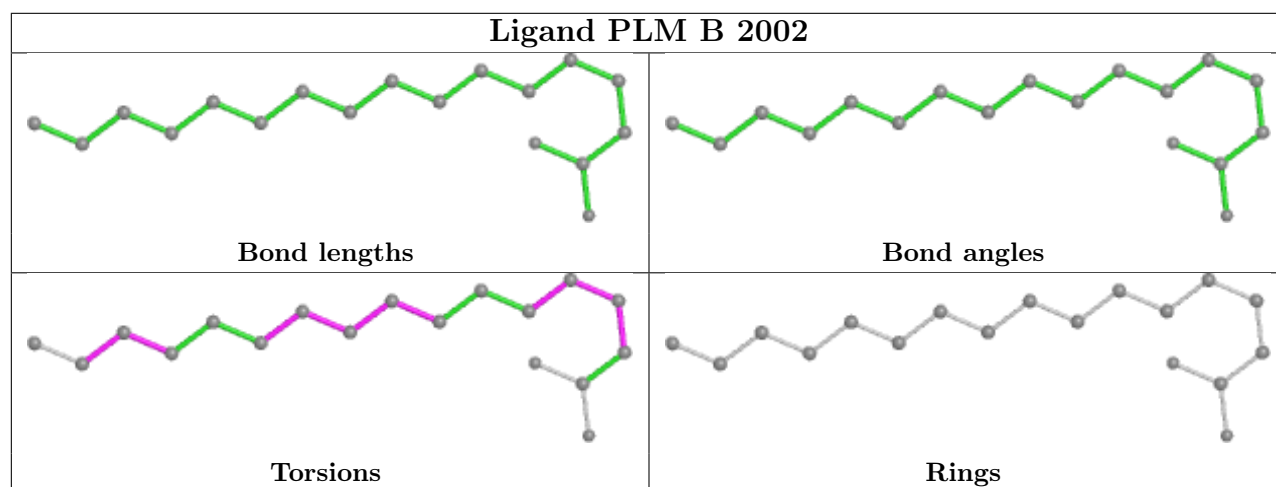
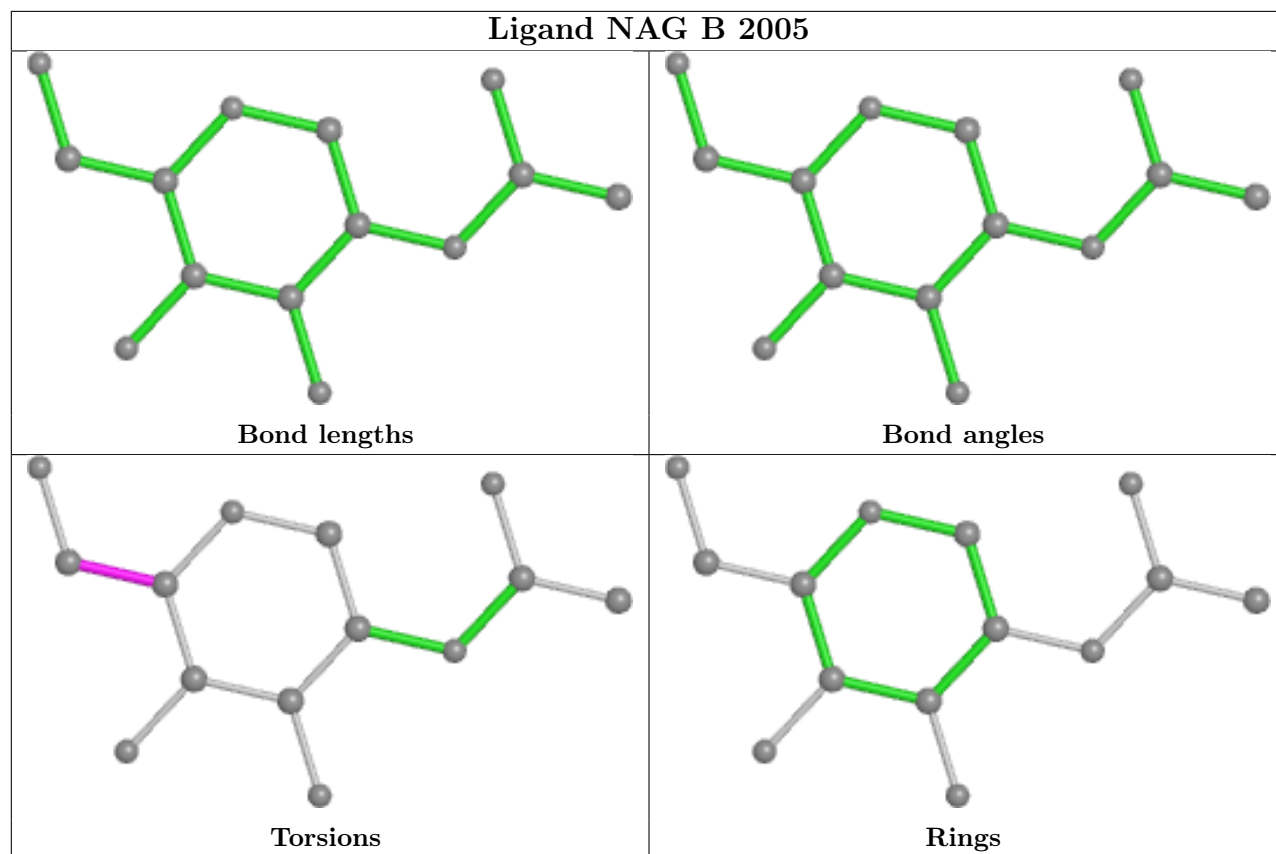
Ligand NAG C 2006

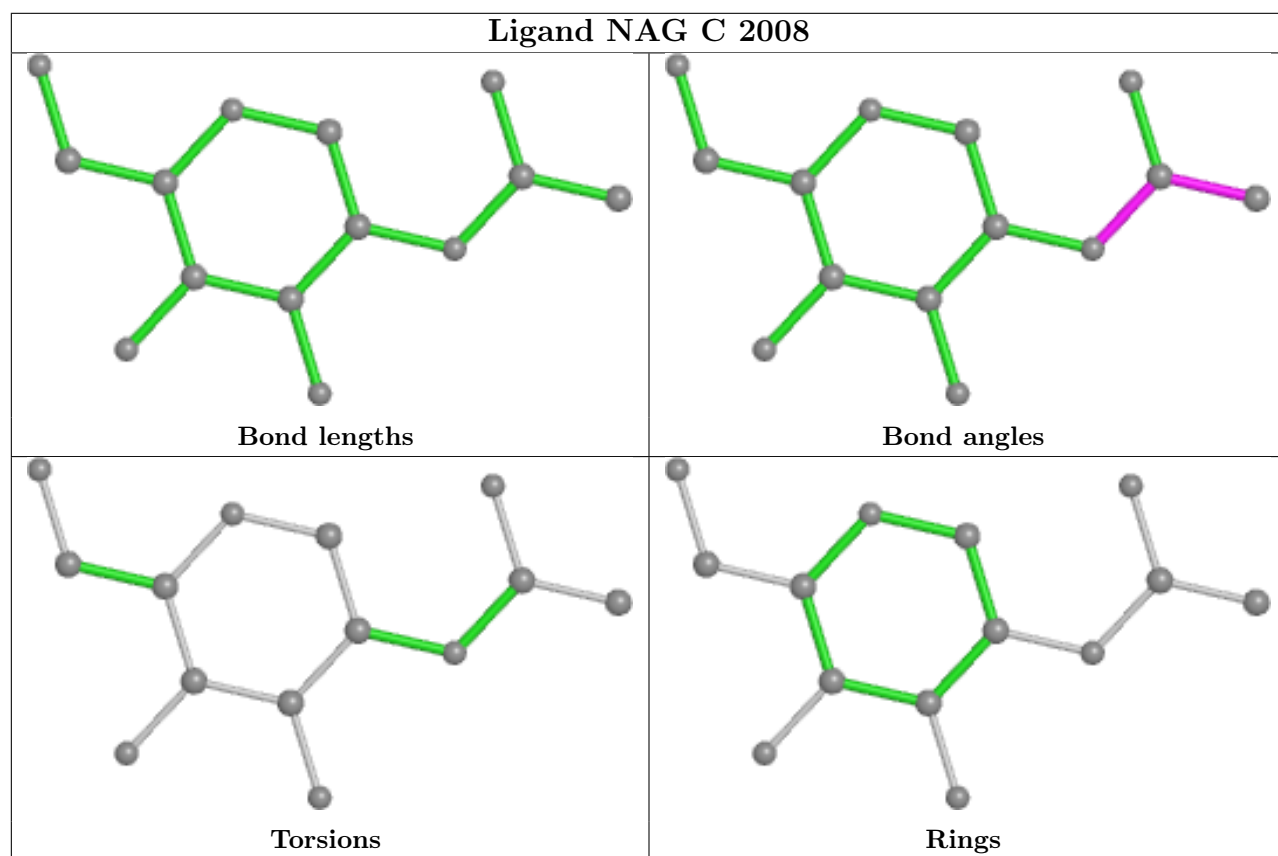
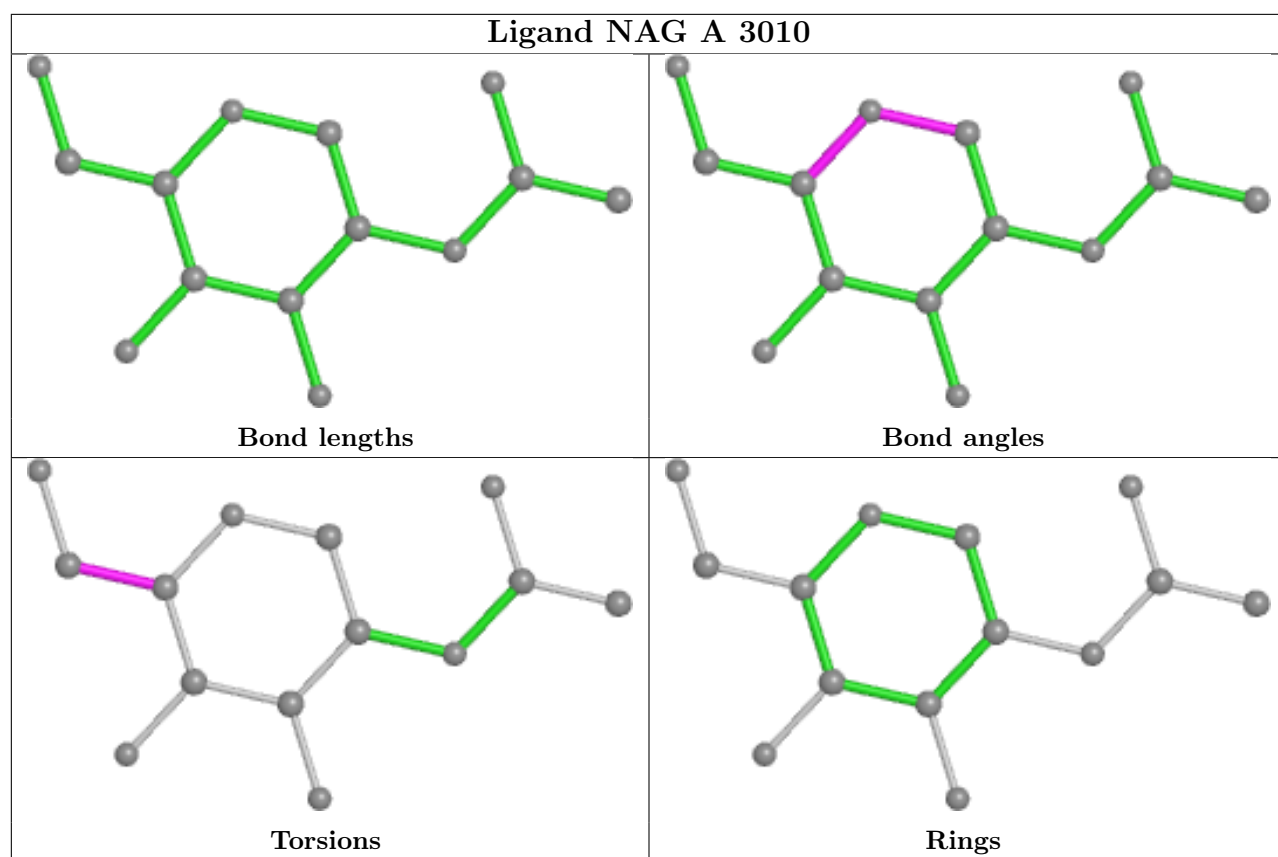


Ligand NAG B 2013





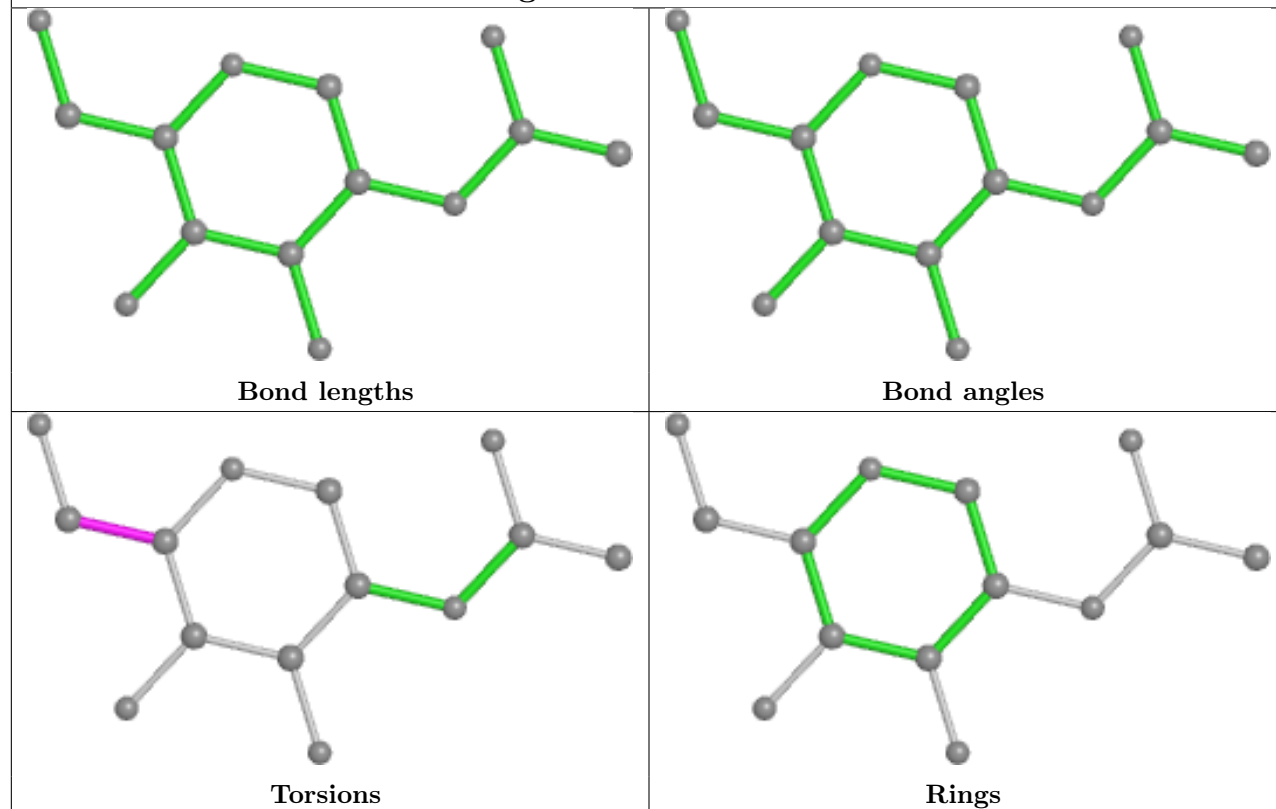




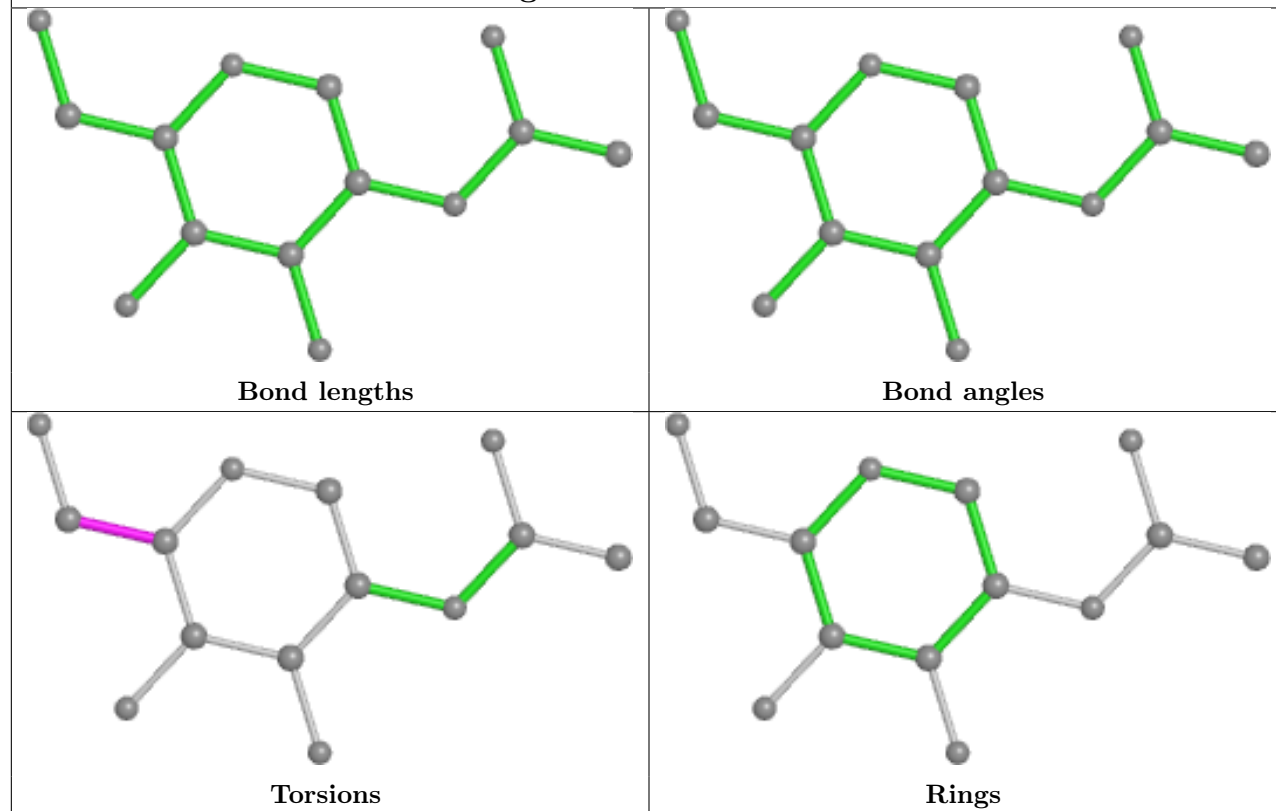
Ligand NAG A 3009



Ligand NAG A 3002

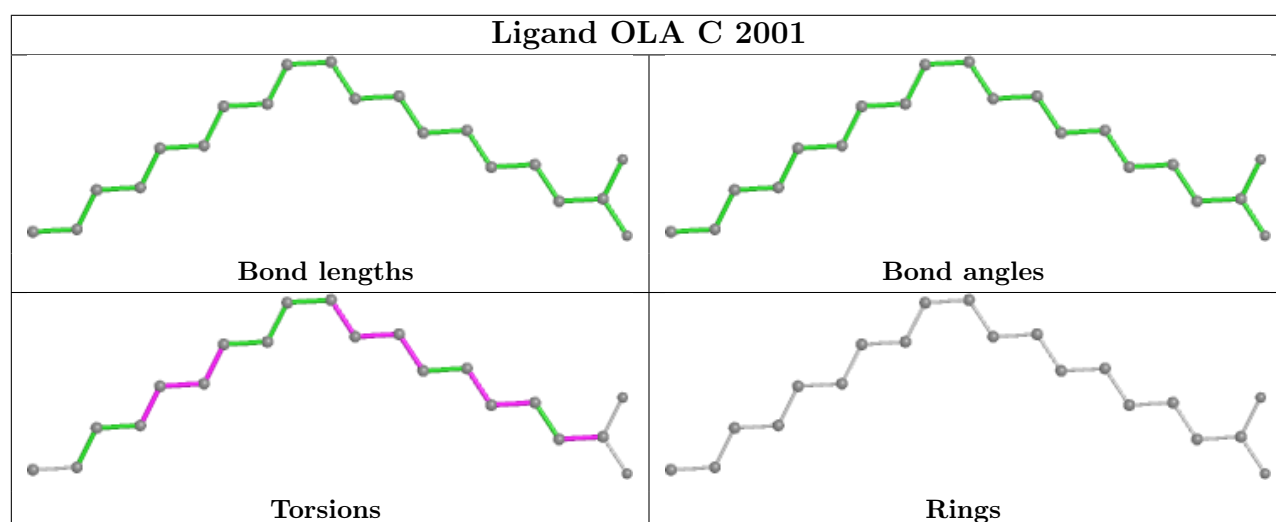
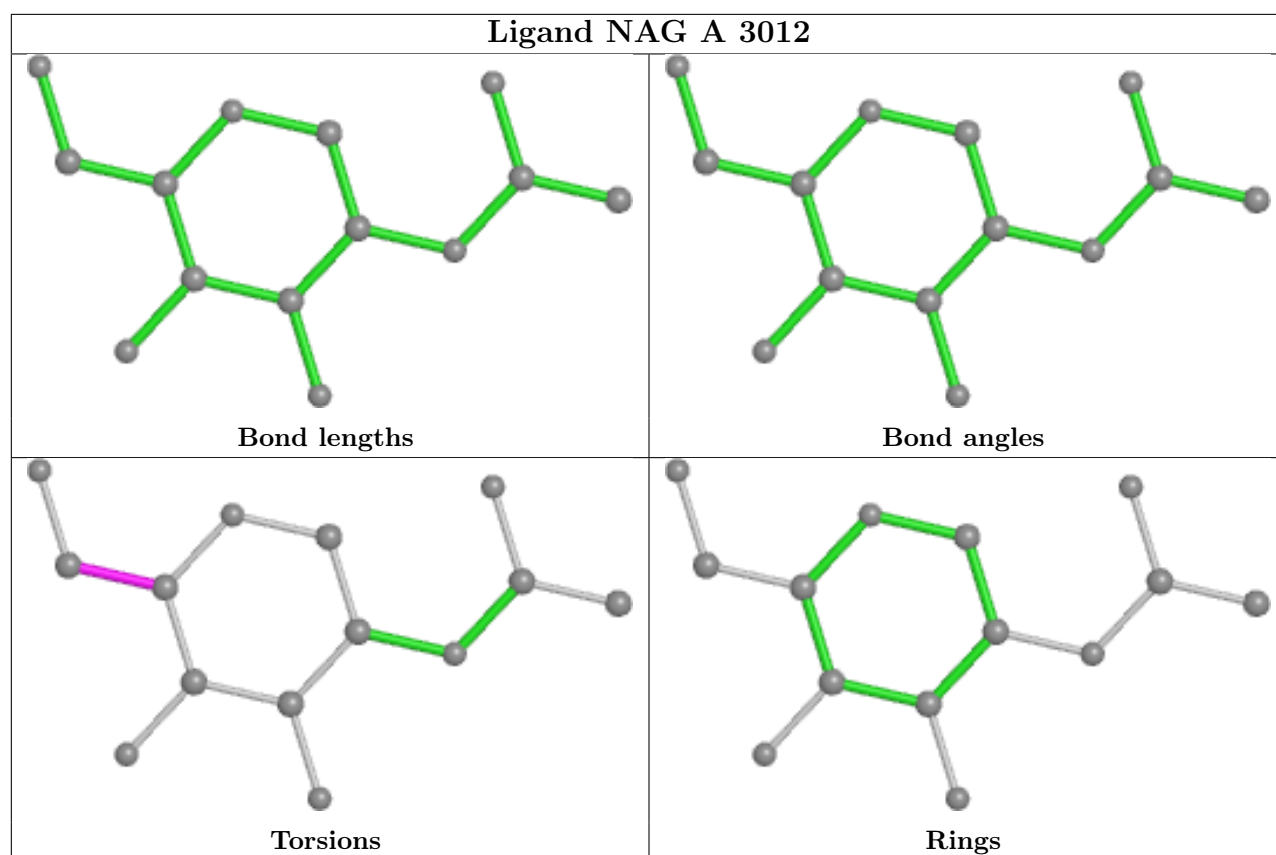


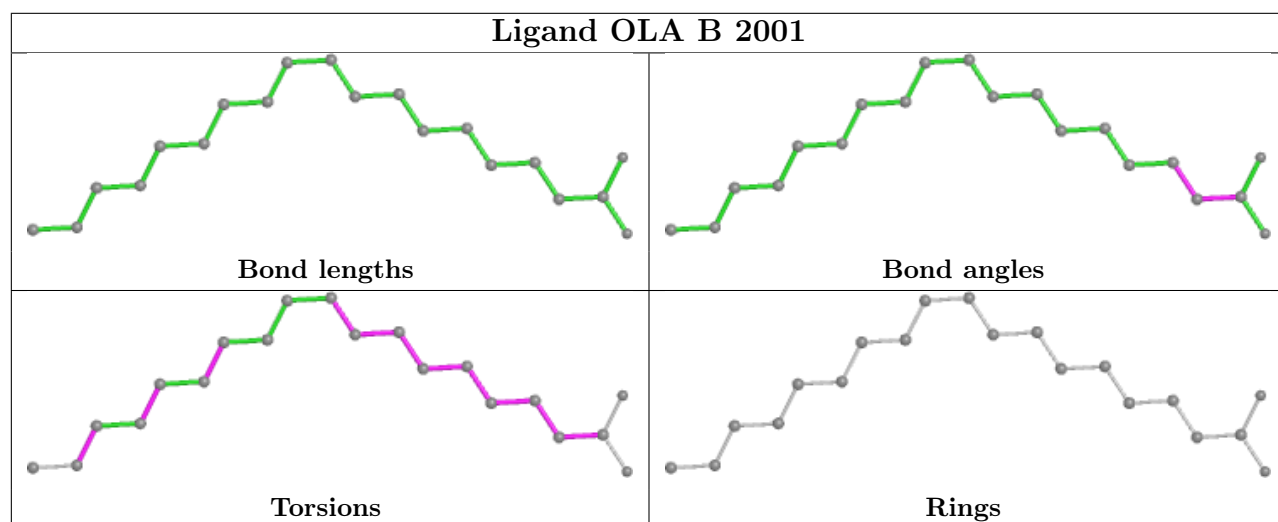
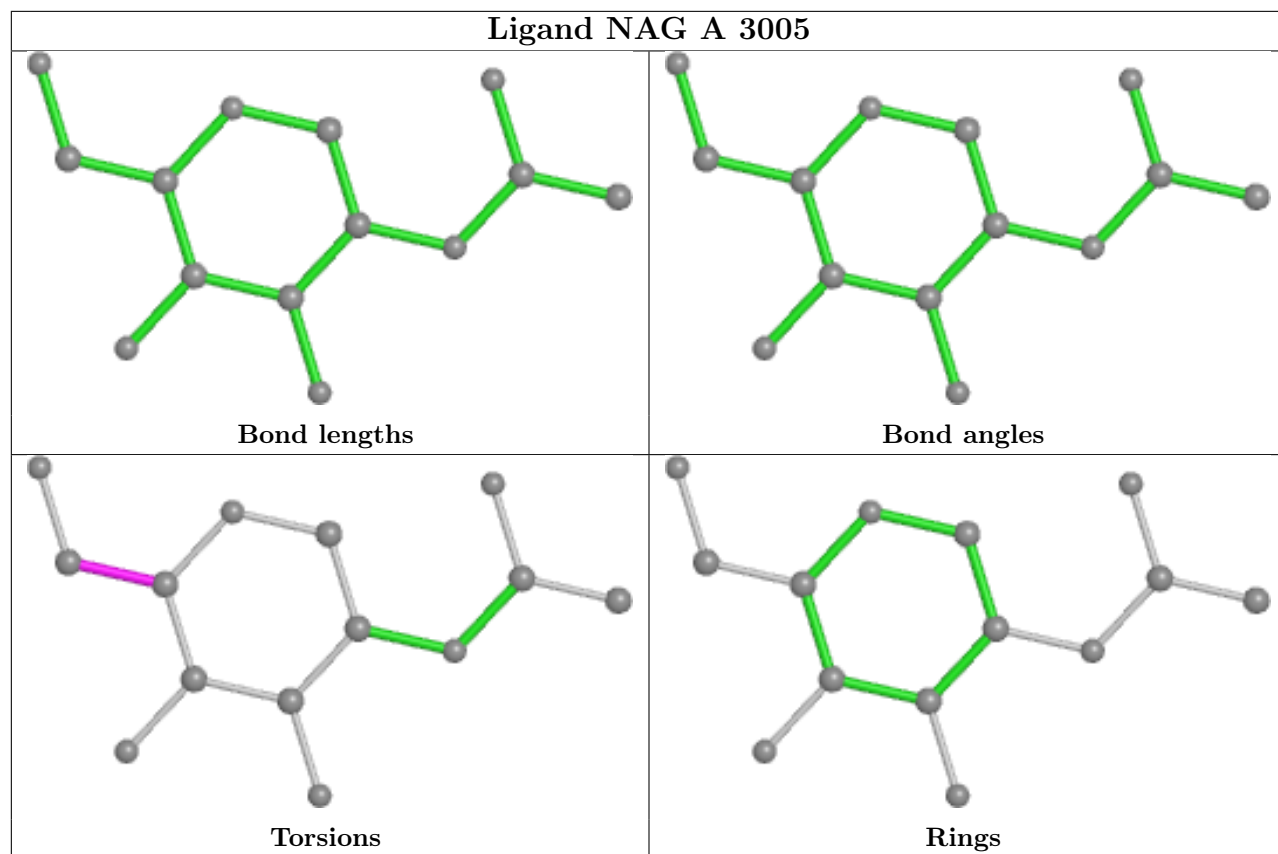
Ligand NAG B 2007

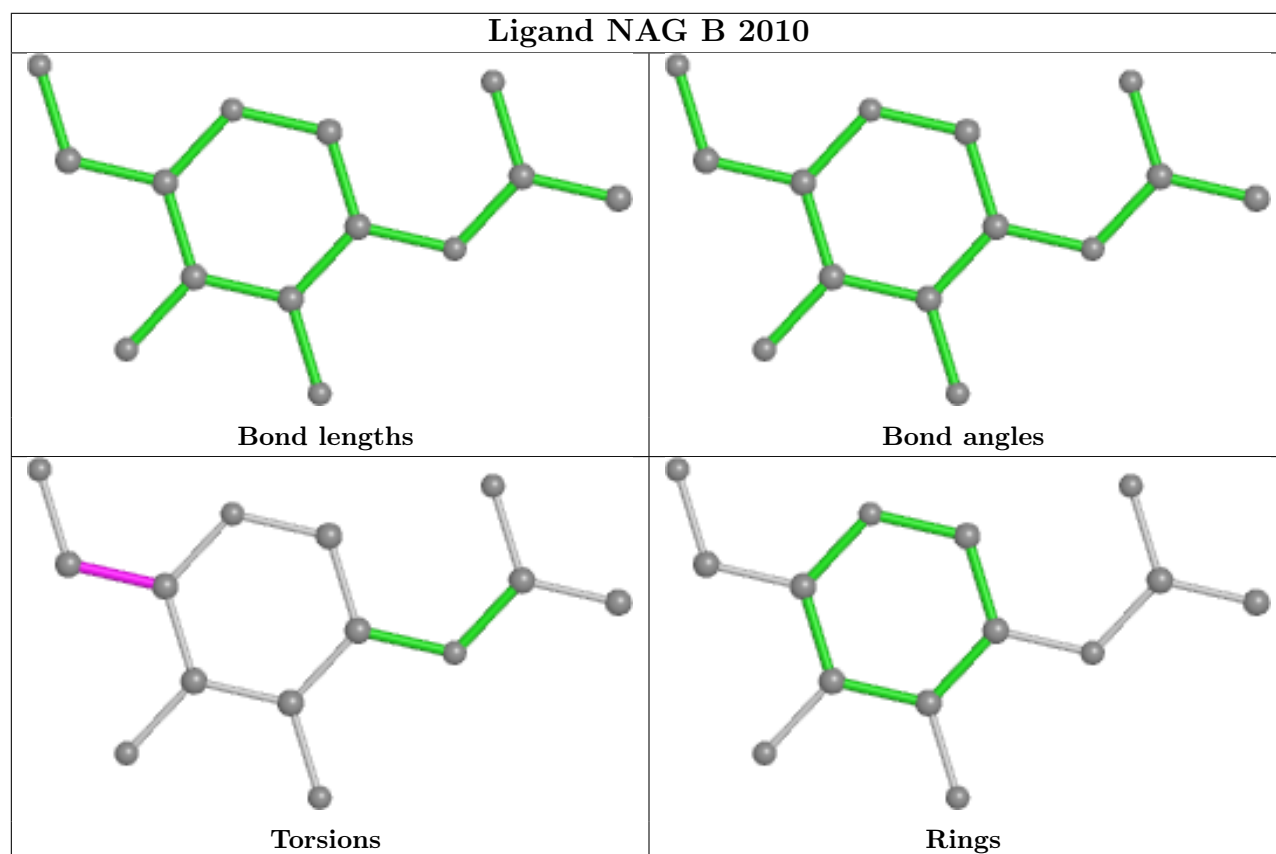
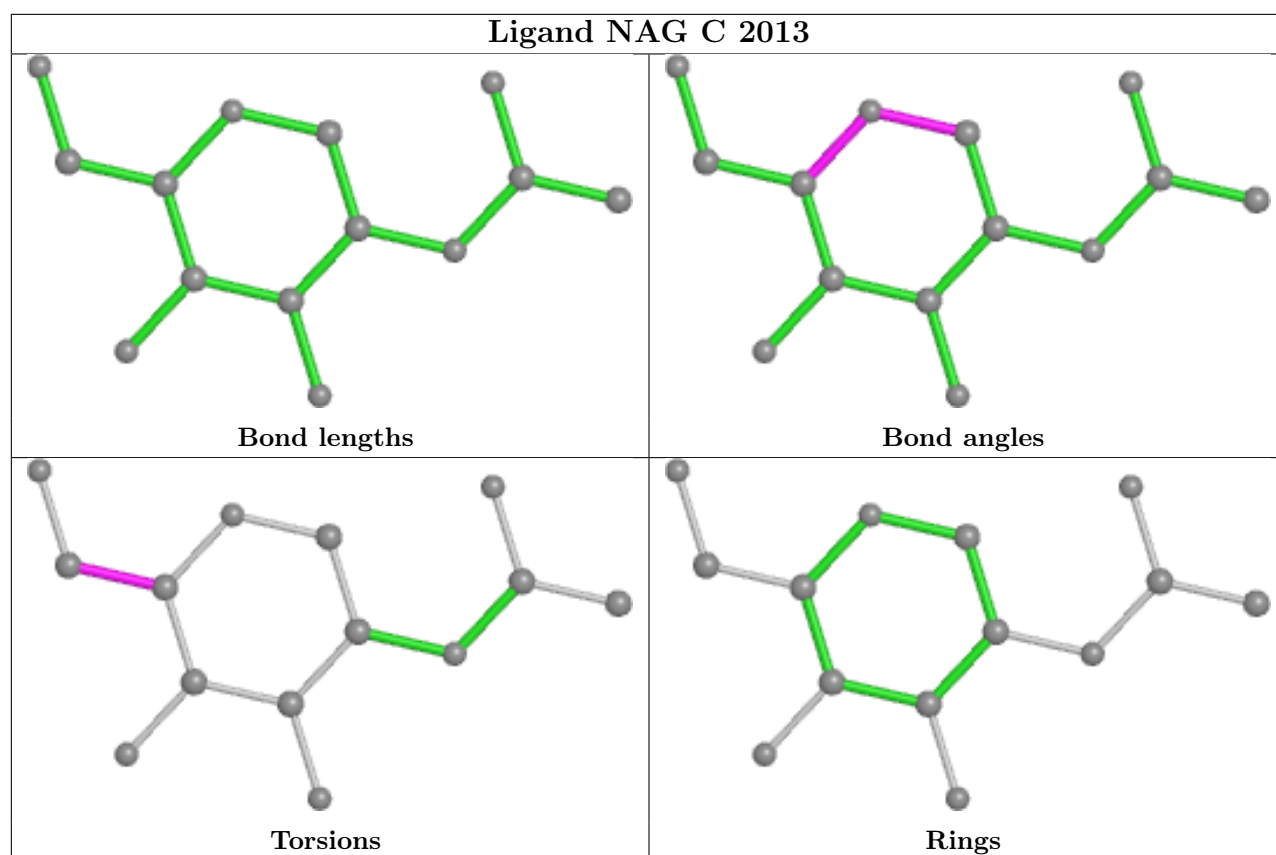


Ligand NAG A 3011

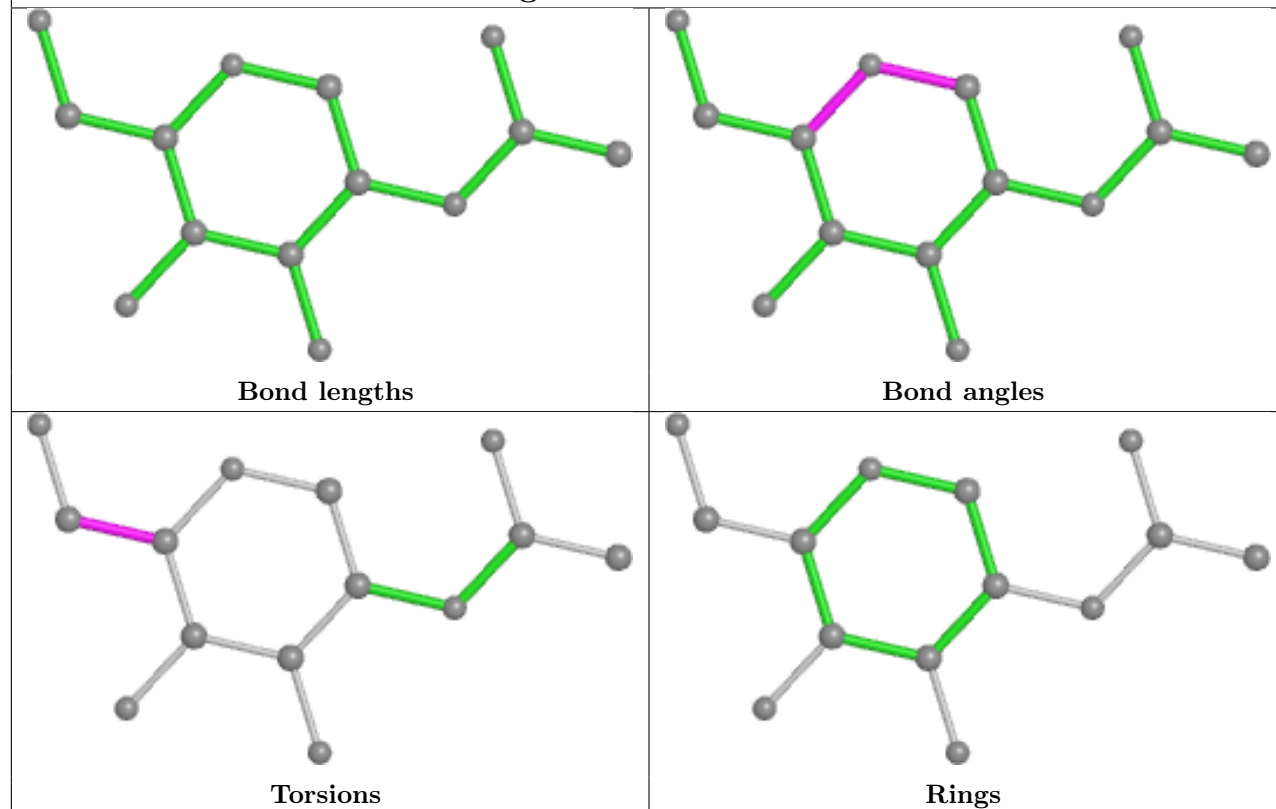




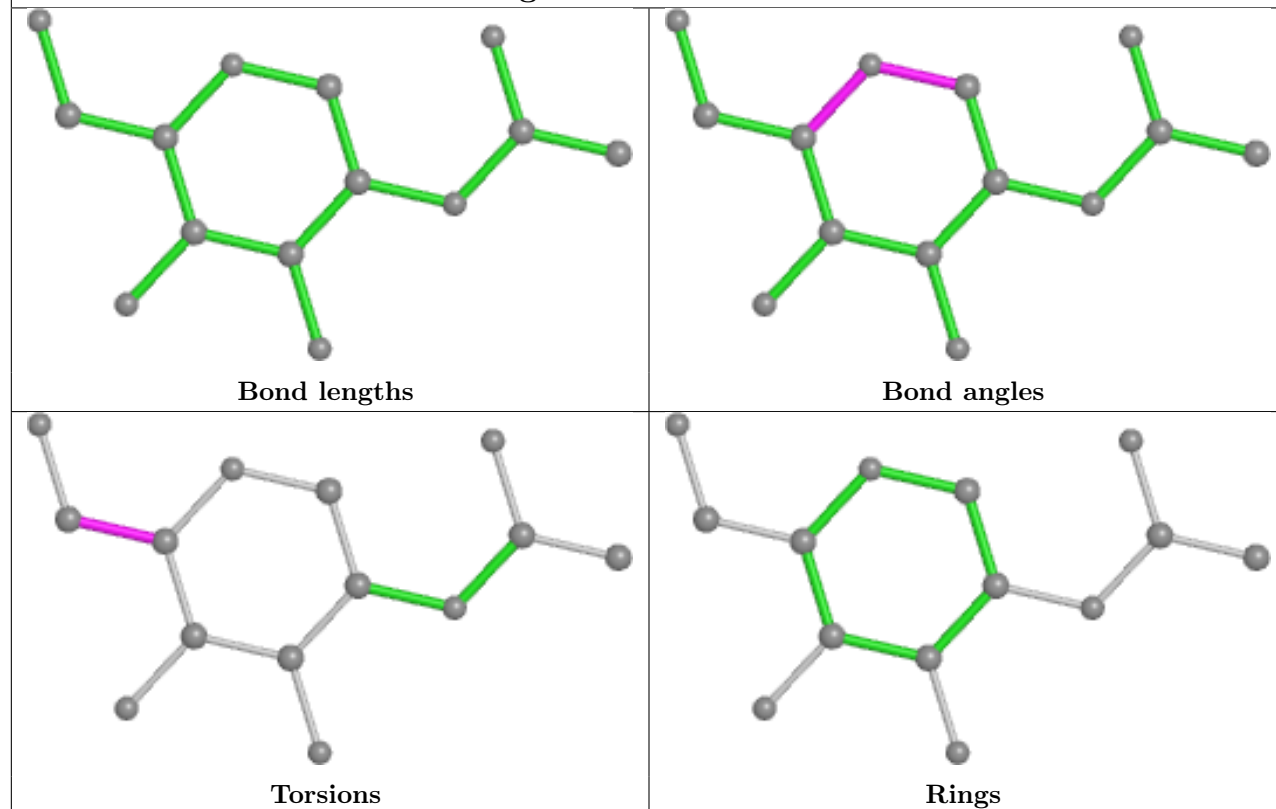


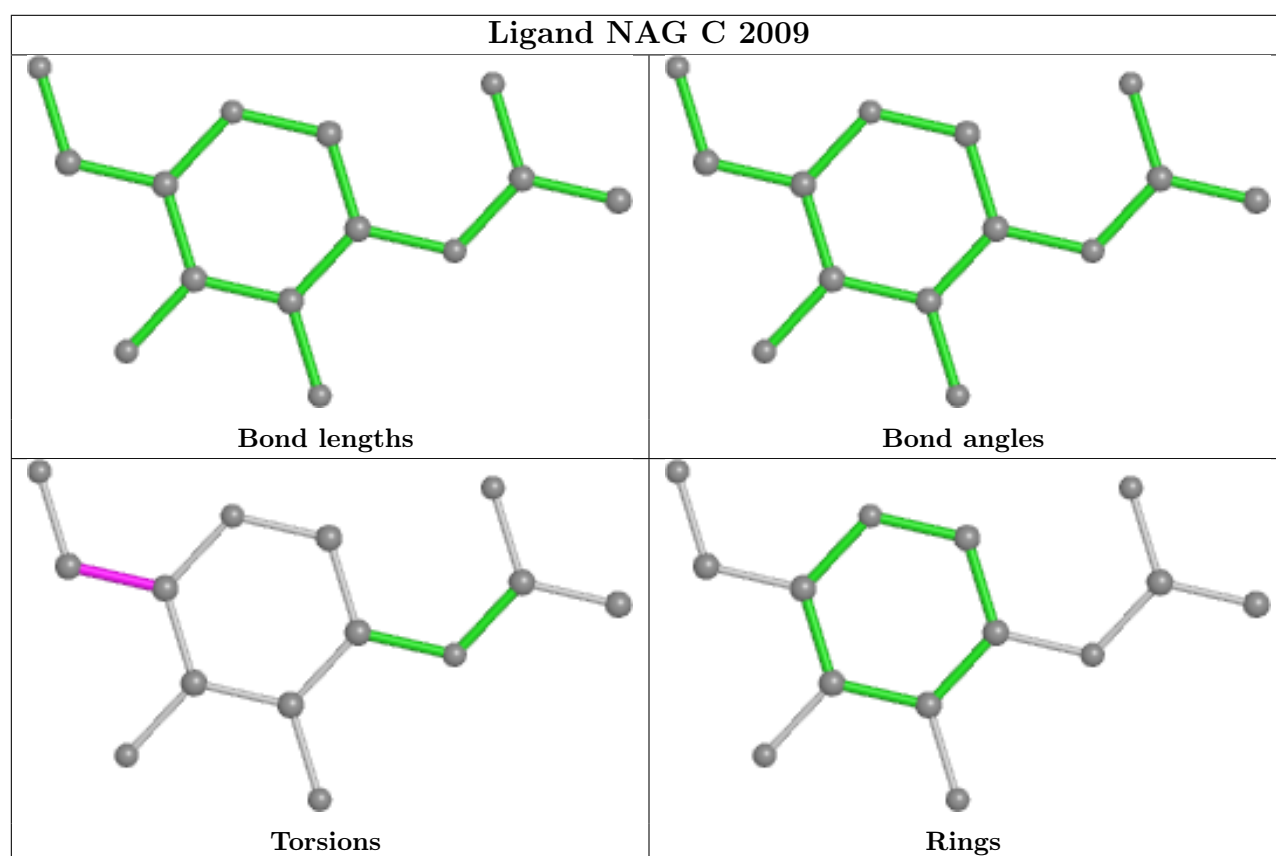
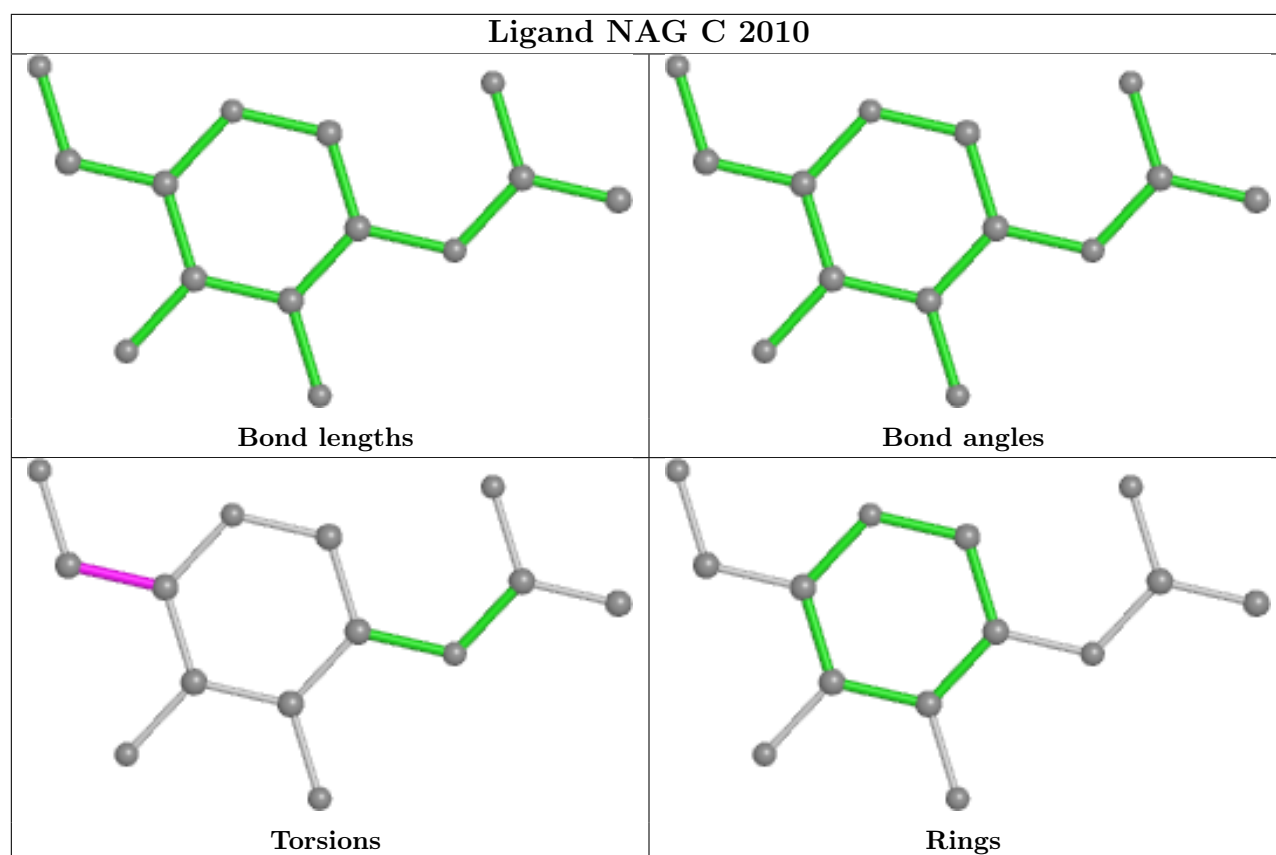


Ligand NAG B 2003

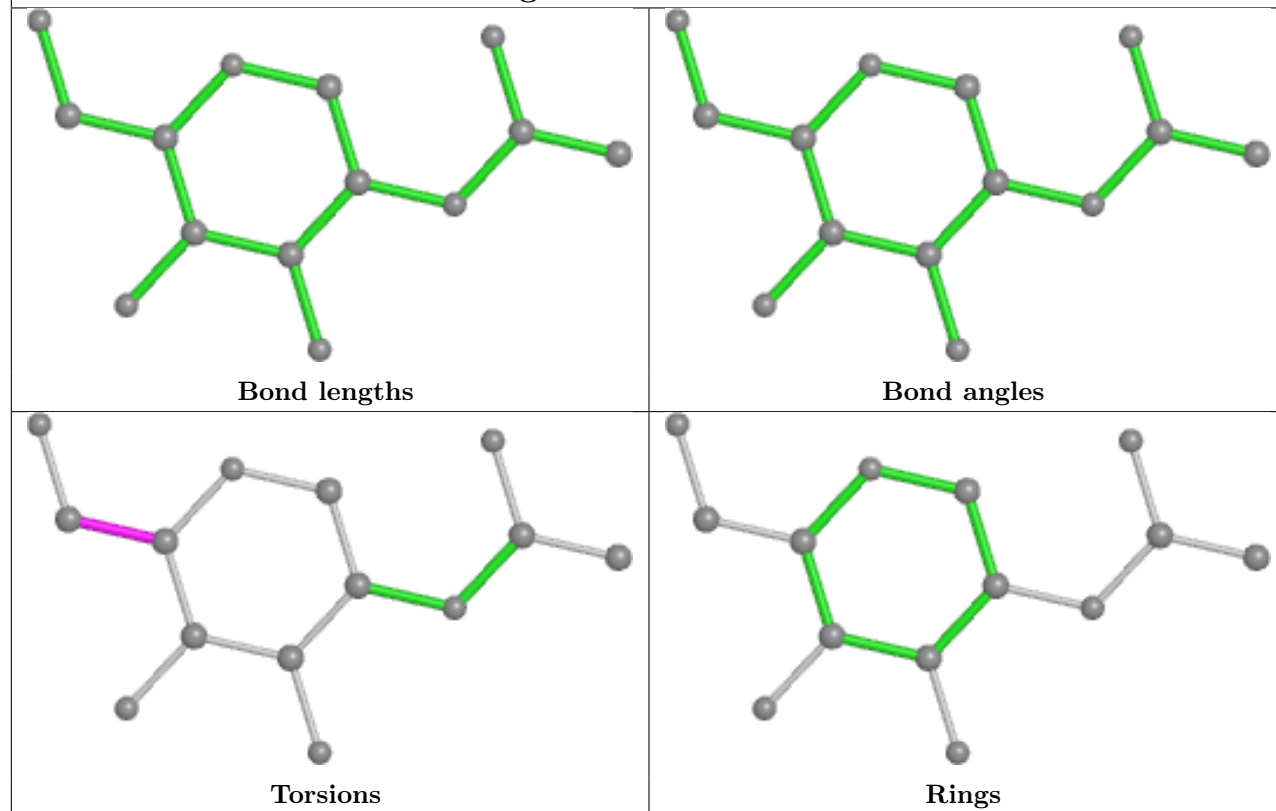


Ligand NAG C 2012

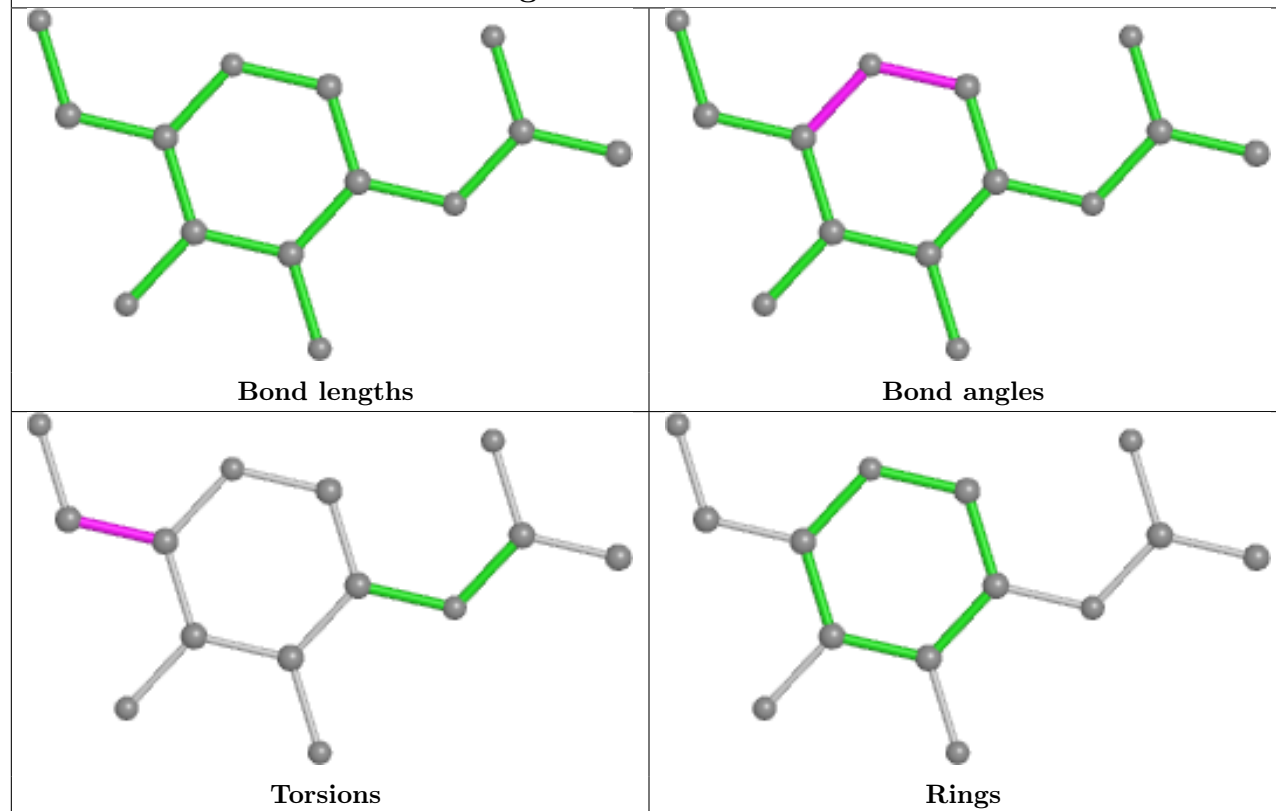




Ligand NAG B 2009



Ligand NAG C 2003



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.

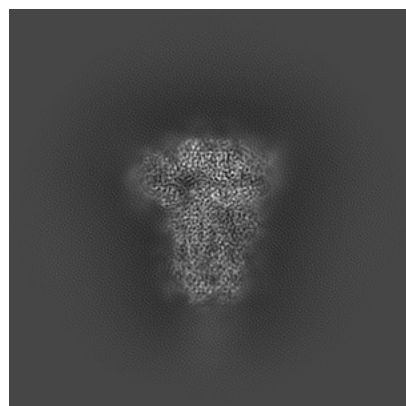
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62522. These allow visual inspection of the internal detail of the map and identification of artifacts.

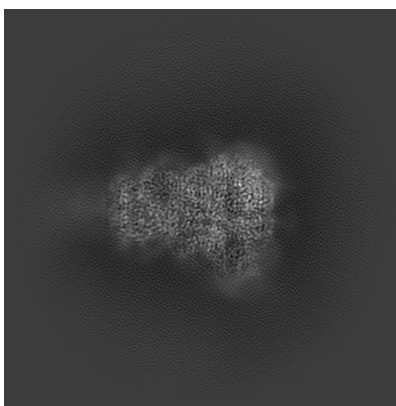
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

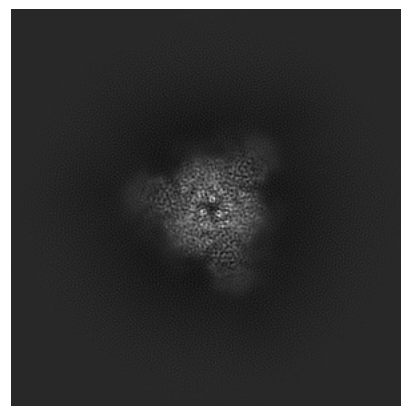
6.1.1 Primary map



X

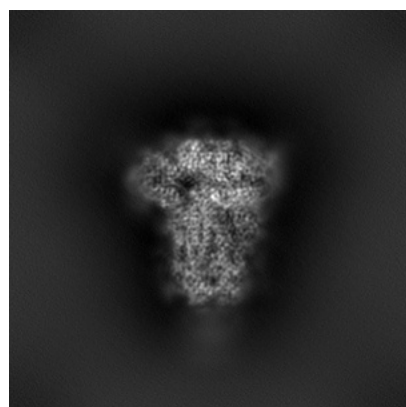


Y

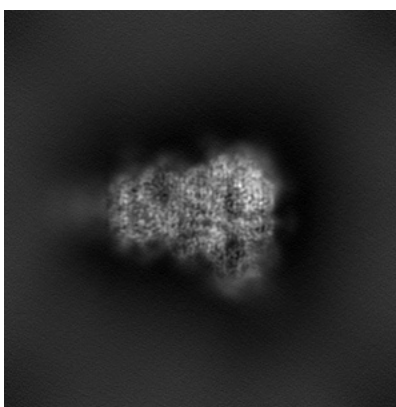


Z

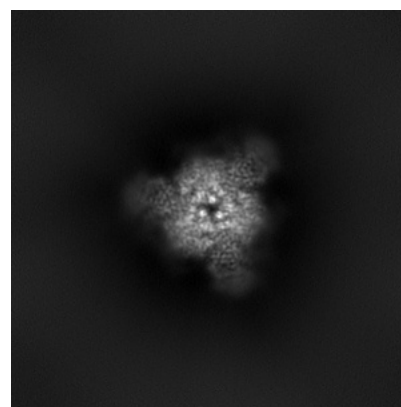
6.1.2 Raw map



X



Y

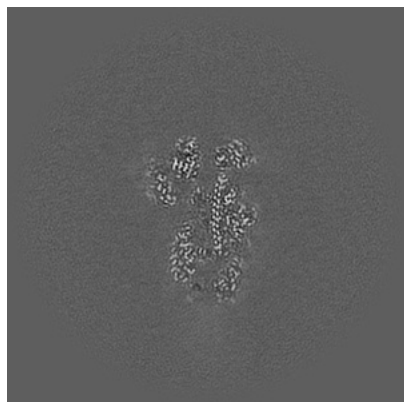


Z

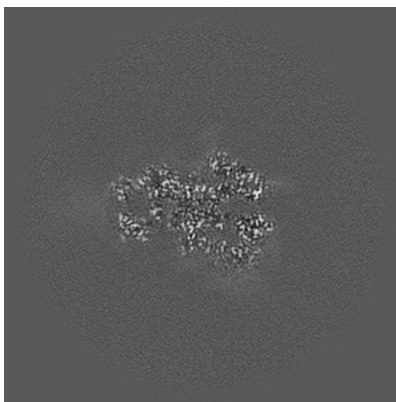
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

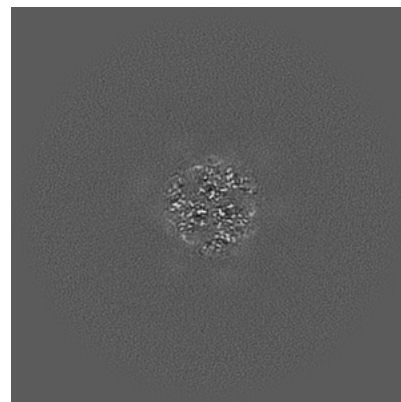
6.2.1 Primary map



X Index: 160

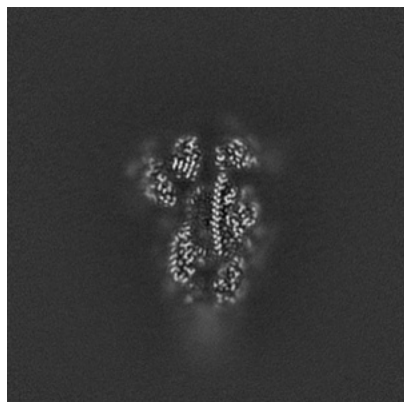


Y Index: 160

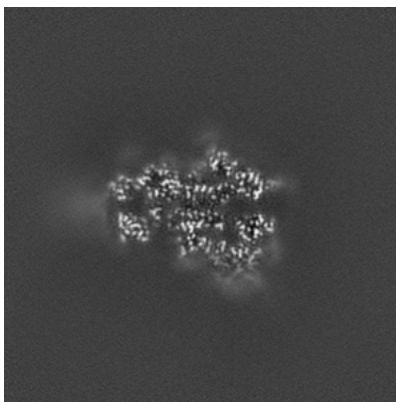


Z Index: 160

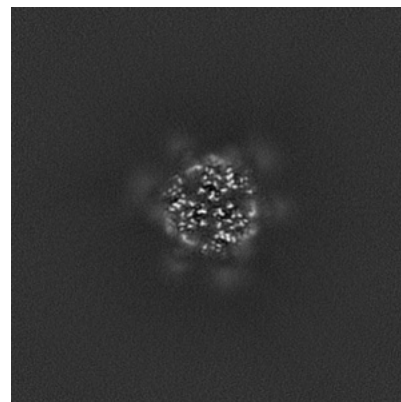
6.2.2 Raw map



X Index: 160



Y Index: 160

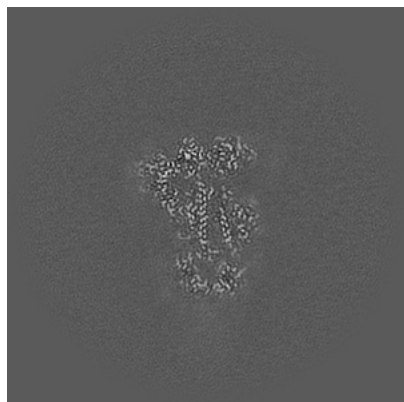


Z Index: 160

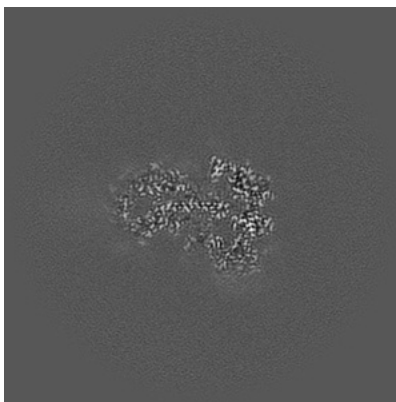
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

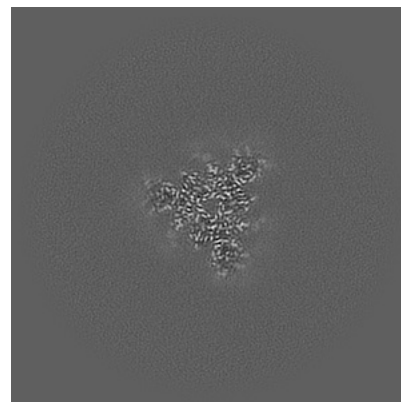
6.3.1 Primary map



X Index: 166

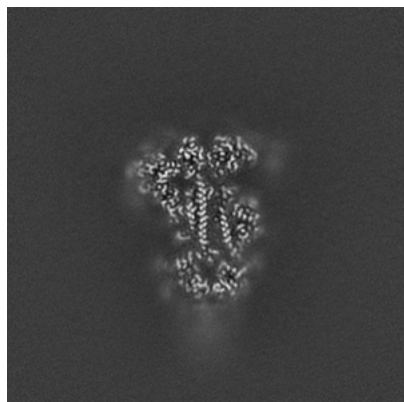


Y Index: 167

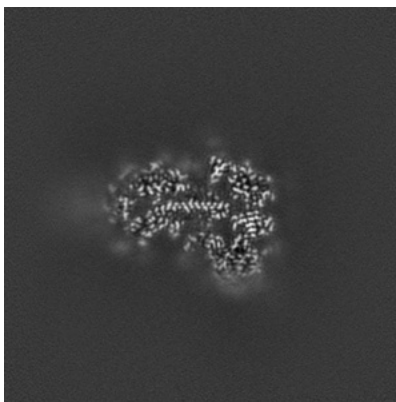


Z Index: 194

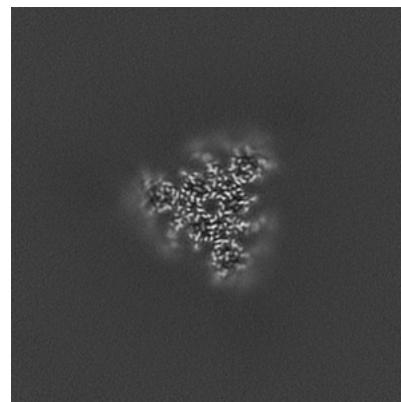
6.3.2 Raw map



X Index: 166



Y Index: 167

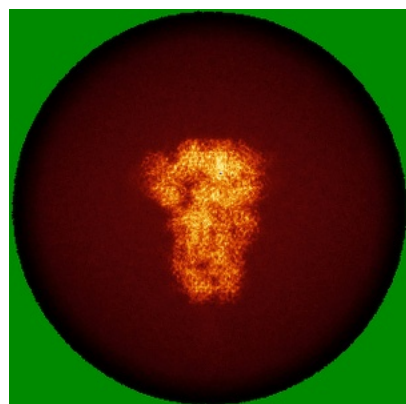


Z Index: 194

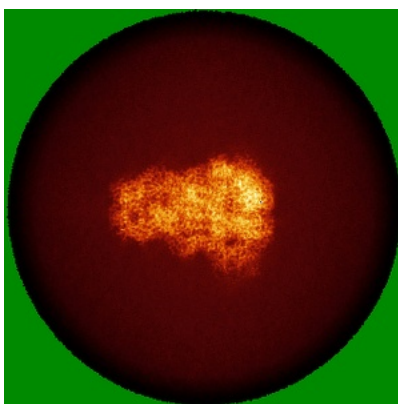
The images above show the largest variance slices of the map in three orthogonal directions.

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

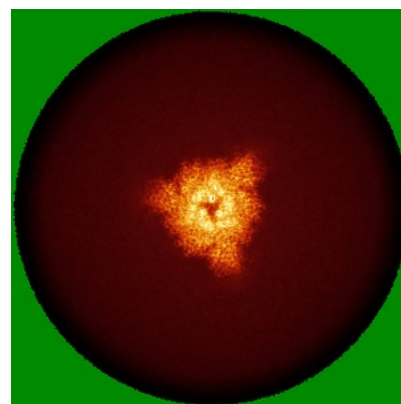
6.4.1 Primary map



X

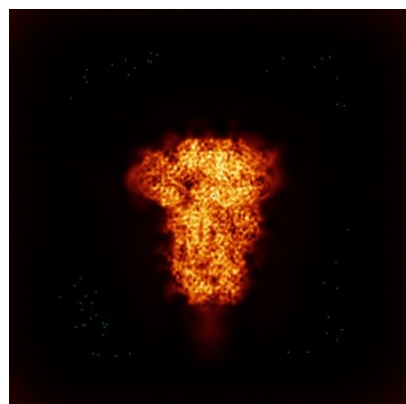


Y

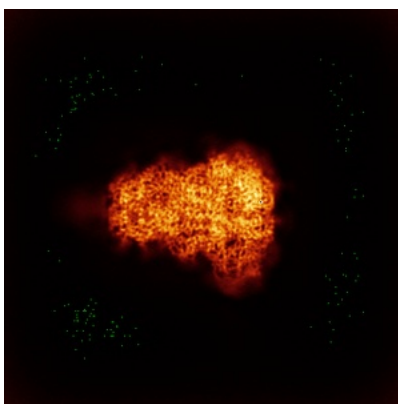


Z

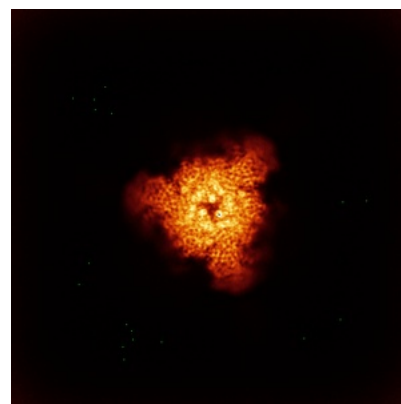
6.4.2 Raw map



X



Y

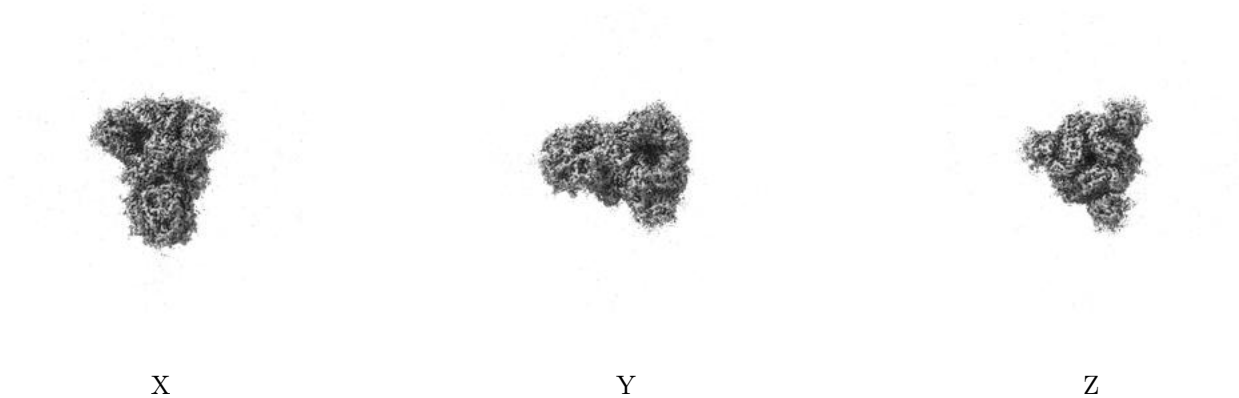


Z

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

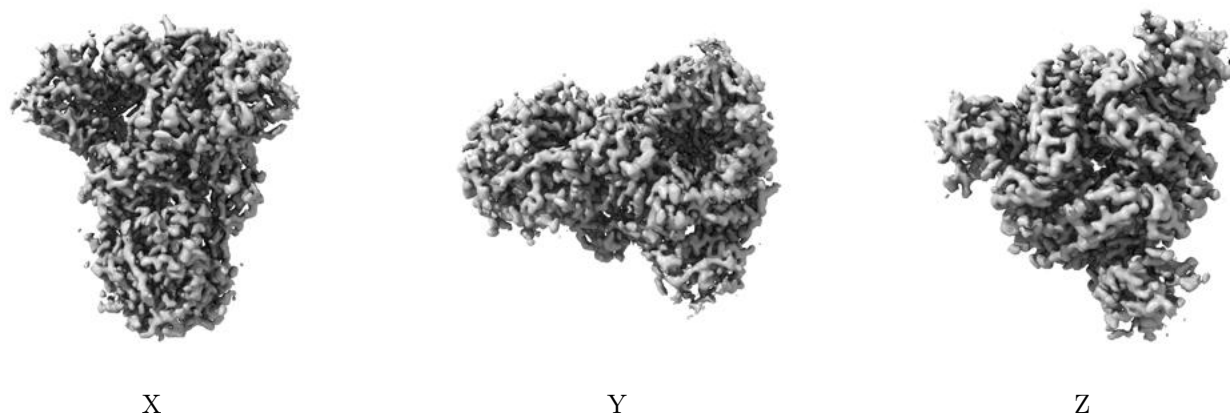
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

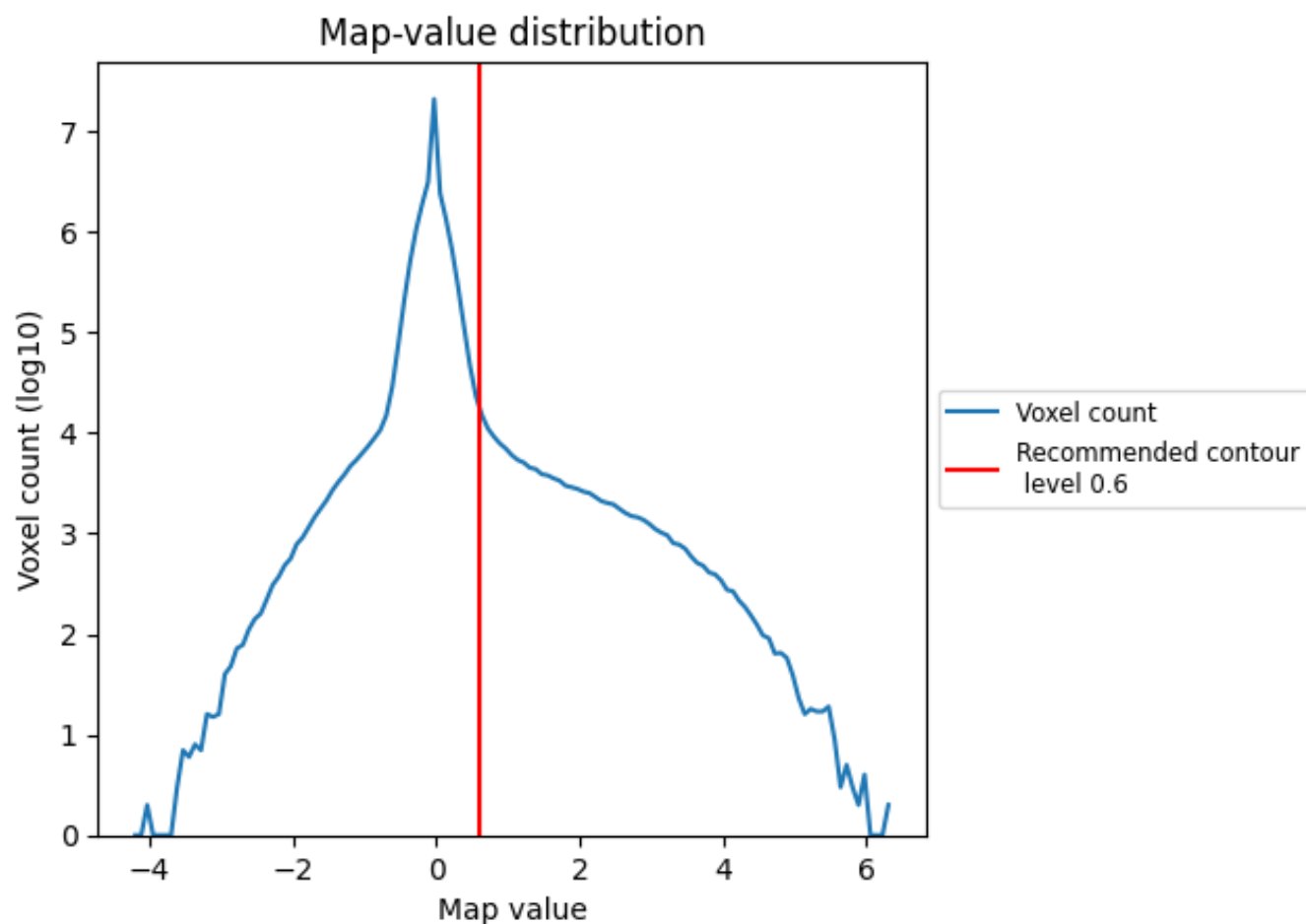
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

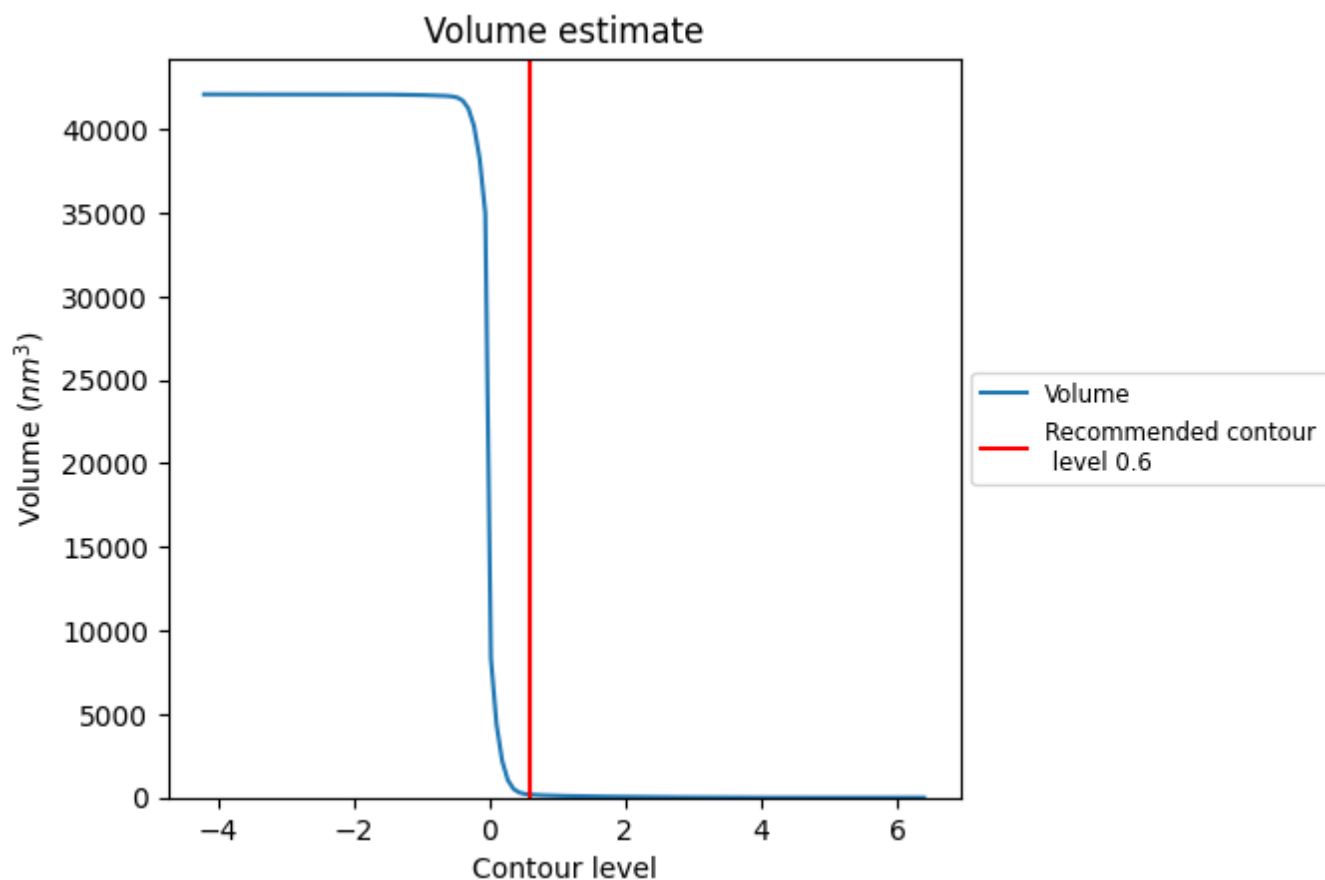
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

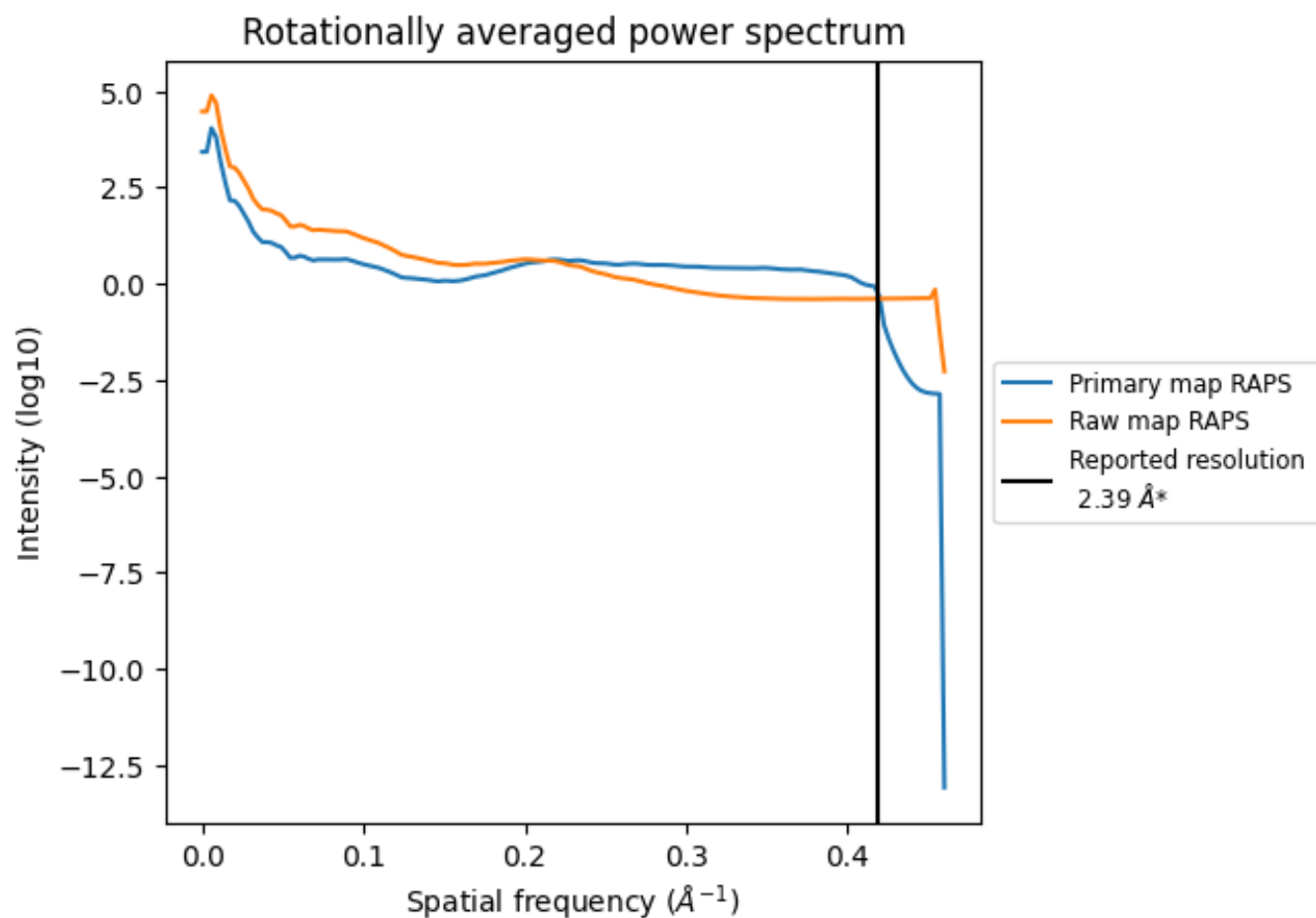
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm^3 ; this corresponds to an approximate mass of 163 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 ⓘ

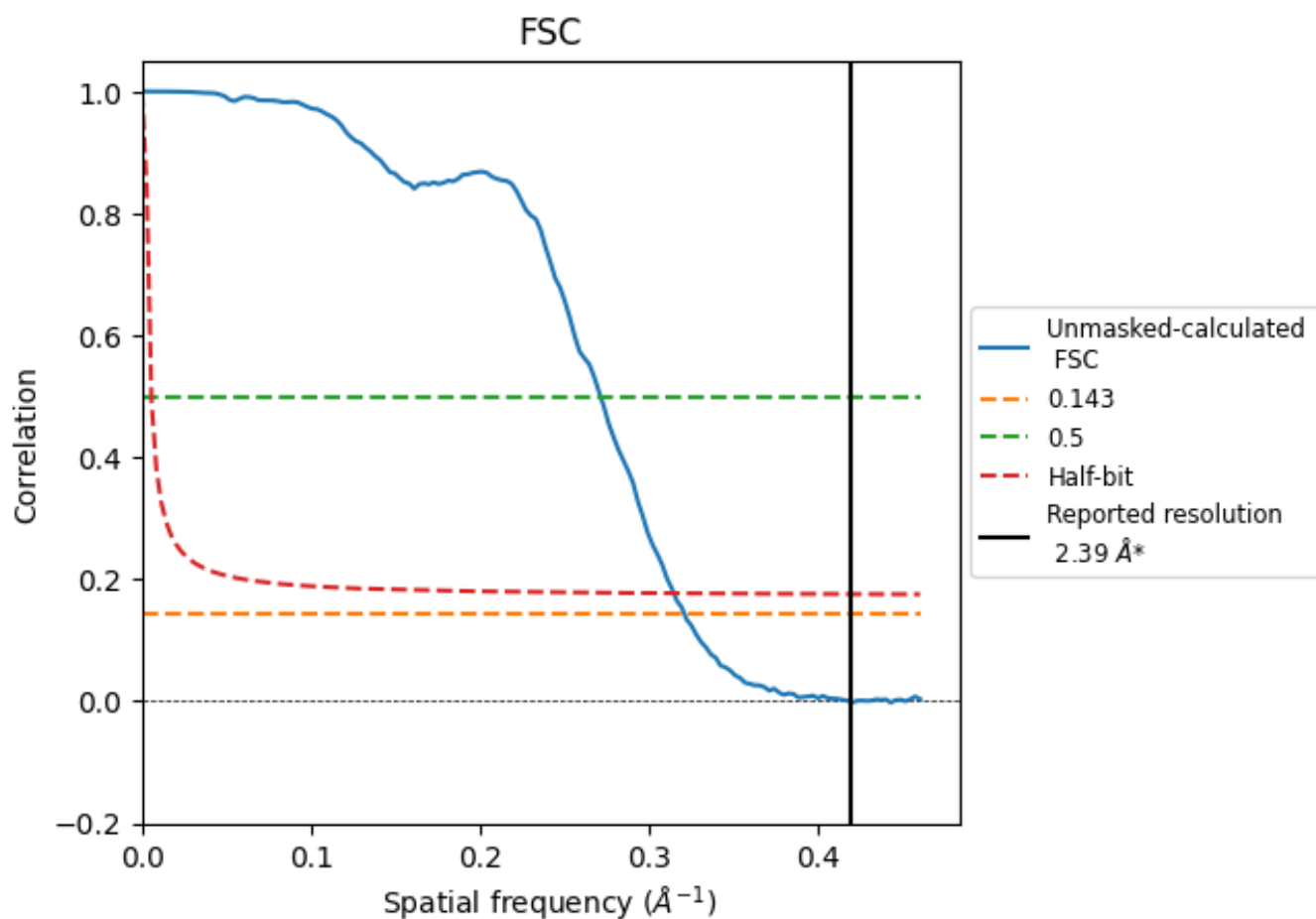


*Reported resolution corresponds to spatial frequency of 0.418 Å⁻¹

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 0.418 \AA^{-1}

8.2 Resolution estimates [i](#)

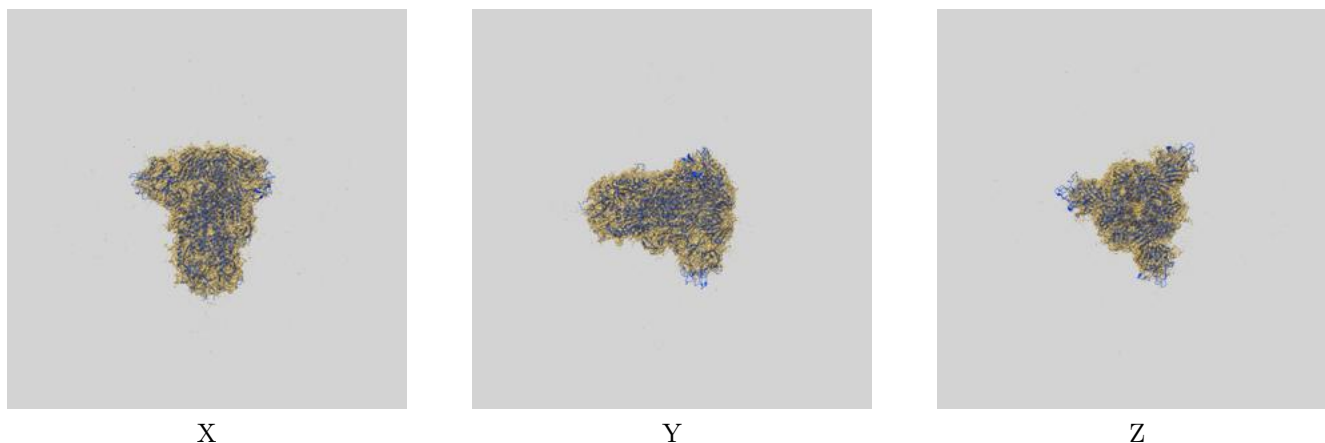
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.12	3.69	3.18

*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 3.12 differs from the reported value 2.39 by more than 10 %

9 Map-model fit [i](#)

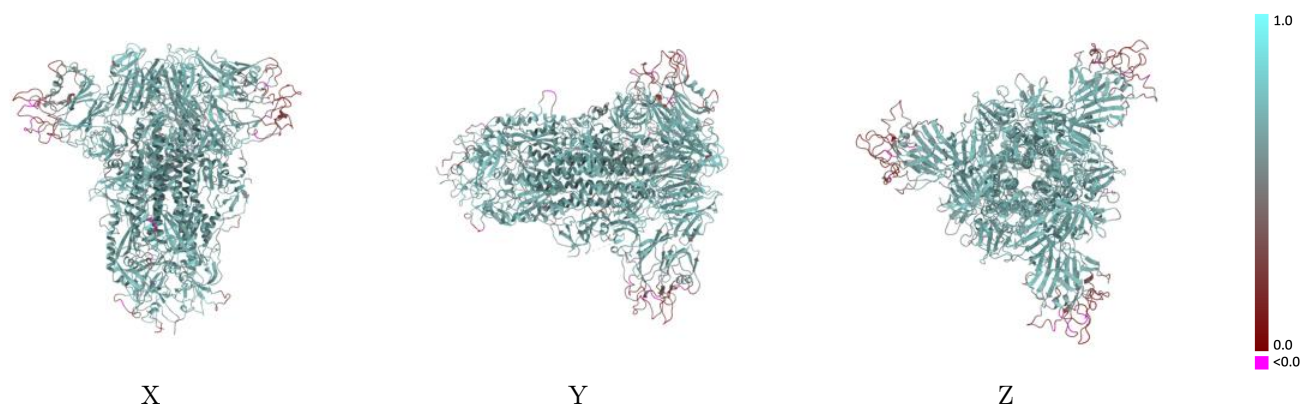
This section contains information regarding the fit between EMDB map EMD-62522 and PDB model 9KR8. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.6 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](#)



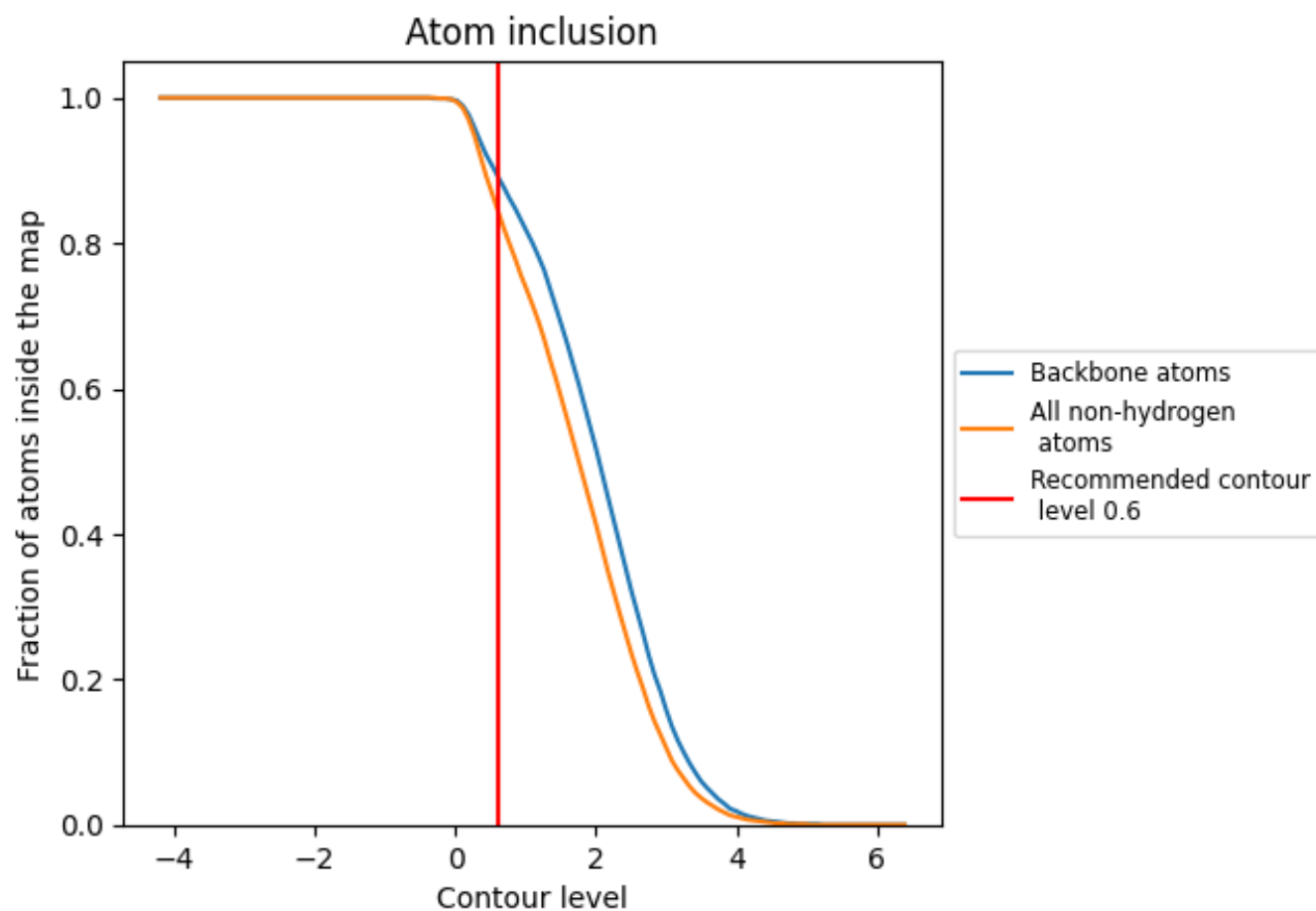
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 85% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.6150
A	 0.8560	 0.6200
B	 0.8560	 0.6160
C	 0.8430	 0.6170
D	 0.7140	 0.5280
E	 0.6070	 0.4780
F	 0.7860	 0.4750
G	 0.4640	 0.4860
H	 0.7860	 0.5350
I	 0.4640	 0.4700
J	 0.5710	 0.5330
K	 0.7860	 0.5810
L	 0.6430	 0.4700
M	 0.6070	 0.4810
N	 0.7500	 0.5060
O	 0.5710	 0.5230
P	 0.7860	 0.5290
Q	 0.3570	 0.4510
R	 0.5000	 0.4890
S	 0.8570	 0.6020
T	 0.6790	 0.5600
U	 0.5000	 0.4090
V	 0.7860	 0.5000
W	 0.5360	 0.5560
X	 0.7500	 0.5530
Y	 0.3930	 0.4070
Z	 0.5360	 0.4470
a	 0.8570	 0.5790

