



Full wwPDB EM Validation Report ⓘ

Oct 26, 2025 – 04:28 AM JST

PDB ID : 9KR9 / pdb_00009kr9
EMDB ID : EMD-62523
Title : Overall structure of HKU5 S protein with S468A/Y463A mutation
Authors : Zhang, Y.Y.; Xia, L.Y.; Zhou, Q.
Deposited on : 2024-11-27
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

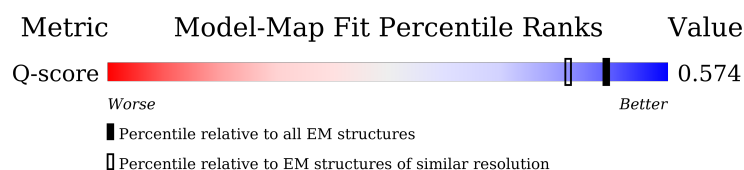
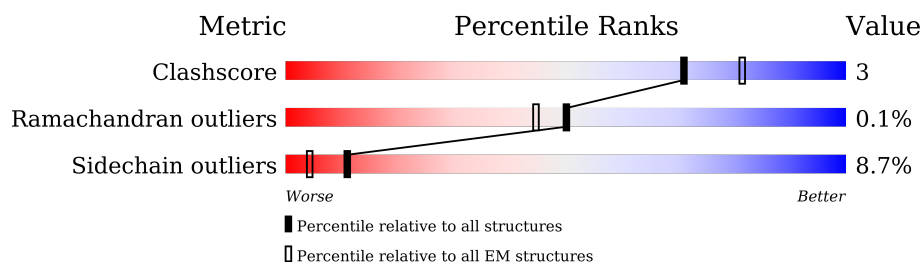
1 Overall quality at a glance

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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
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	1352	<div> <div>7%</div> <div>75%</div> <div>11%</div> <div>12%</div> </div>
1	B	1352	<div> <div>7%</div> <div>75%</div> <div>11%</div> <div>12%</div> </div>
1	C	1352	<div> <div>7%</div> <div>75%</div> <div>11%</div> <div>12%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>

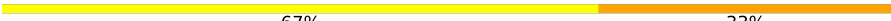
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Mol	Chain	Length	Quality of chain
2	E	2	<div> <div>50%</div> <div>100%</div> </div>
2	F	2	<div> <div>50%</div> <div>50%</div> </div>
2	H	2	<div> <div>50%</div> <div>100%</div> </div>
2	I	2	<div> <div>100%</div> </div>
2	J	2	<div> <div>50%</div> <div>50%</div> </div>
2	K	2	<div> <div>50%</div> <div>100%</div> </div>
2	L	2	<div> <div>50%</div> <div>50%</div> </div>
2	M	2	<div> <div>50%</div> <div>50%</div> </div>
2	N	2	<div> <div>50%</div> <div>100%</div> </div>
2	O	2	<div> <div>50%</div> <div>50%</div> </div>
2	Q	2	<div> <div>50%</div> <div>100%</div> </div>
2	R	2	<div> <div>100%</div> </div>
2	S	2	<div> <div>50%</div> <div>50%</div> </div>
2	T	2	<div> <div>50%</div> <div>100%</div> </div>
2	U	2	<div> <div>50%</div> <div>50%</div> </div>
2	V	2	<div> <div>50%</div> <div>50%</div> </div>
2	W	2	<div> <div>50%</div> <div>100%</div> </div>
2	X	2	<div> <div>50%</div> <div>50%</div> </div>
2	Z	2	<div> <div>50%</div> <div>100%</div> </div>
2	a	2	<div> <div>100%</div> </div>
2	b	2	<div> <div>50%</div> <div>50%</div> </div>
2	c	2	<div> <div>50%</div> <div>100%</div> </div>
2	d	2	<div> <div>50%</div> <div>50%</div> </div>
3	G	3	<div> <div>67%</div> <div>33%</div> </div>
3	P	3	<div> <div>67%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Y	3	 67% 33%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 28851 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	1184	Total	C	N	O	S	0	0
			9193	5830	1521	1790	52		
1	C	1184	Total	C	N	O	S	0	0
			9193	5830	1521	1790	52		
1	B	1184	Total	C	N	O	S	0	0
			9193	5830	1521	1790	52		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	463	ALA	TYR	engineered mutation	UNP A3EXD0
A	468	ALA	SER	engineered mutation	UNP A3EXD0
C	463	ALA	TYR	engineered mutation	UNP A3EXD0
C	468	ALA	SER	engineered mutation	UNP A3EXD0
B	463	ALA	TYR	engineered mutation	UNP A3EXD0
B	468	ALA	SER	engineered mutation	UNP A3EXD0

- 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	H	2	Total	C	N	O	0	0
			28	16	2	10		

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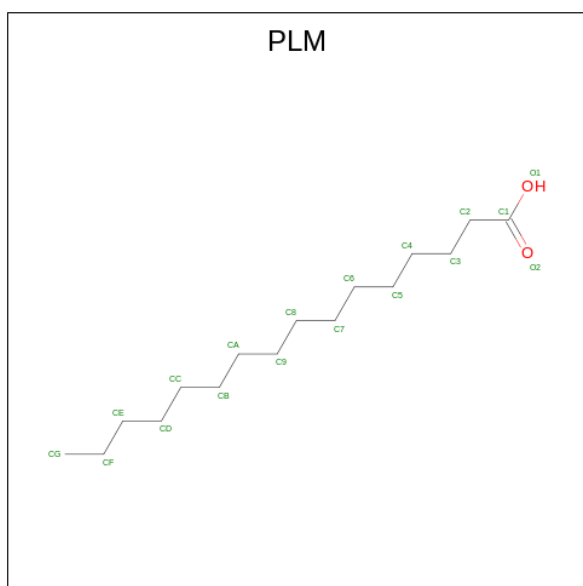
Mol	Chain	Residues	Atoms				AltConf	Trace
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16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

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



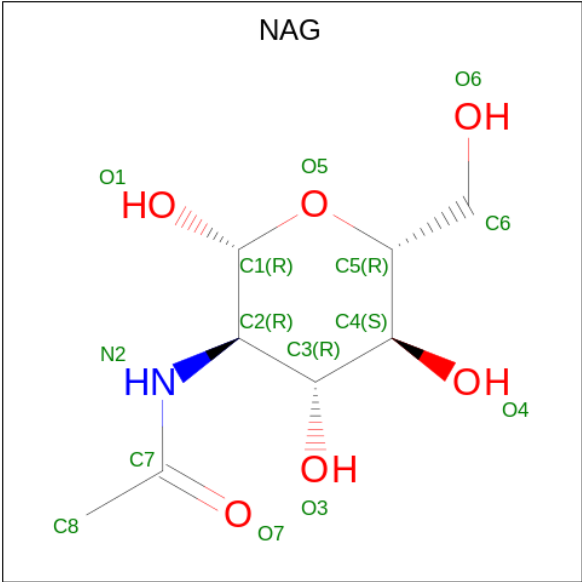
Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	3	Total	C	N	O	0	0
			42	24	3	15		
3	P	3	Total	C	N	O	0	0
			42	24	3	15		
3	Y	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 4 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
4	A	1	Total	C	O	0
			18	16	2	
4	C	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



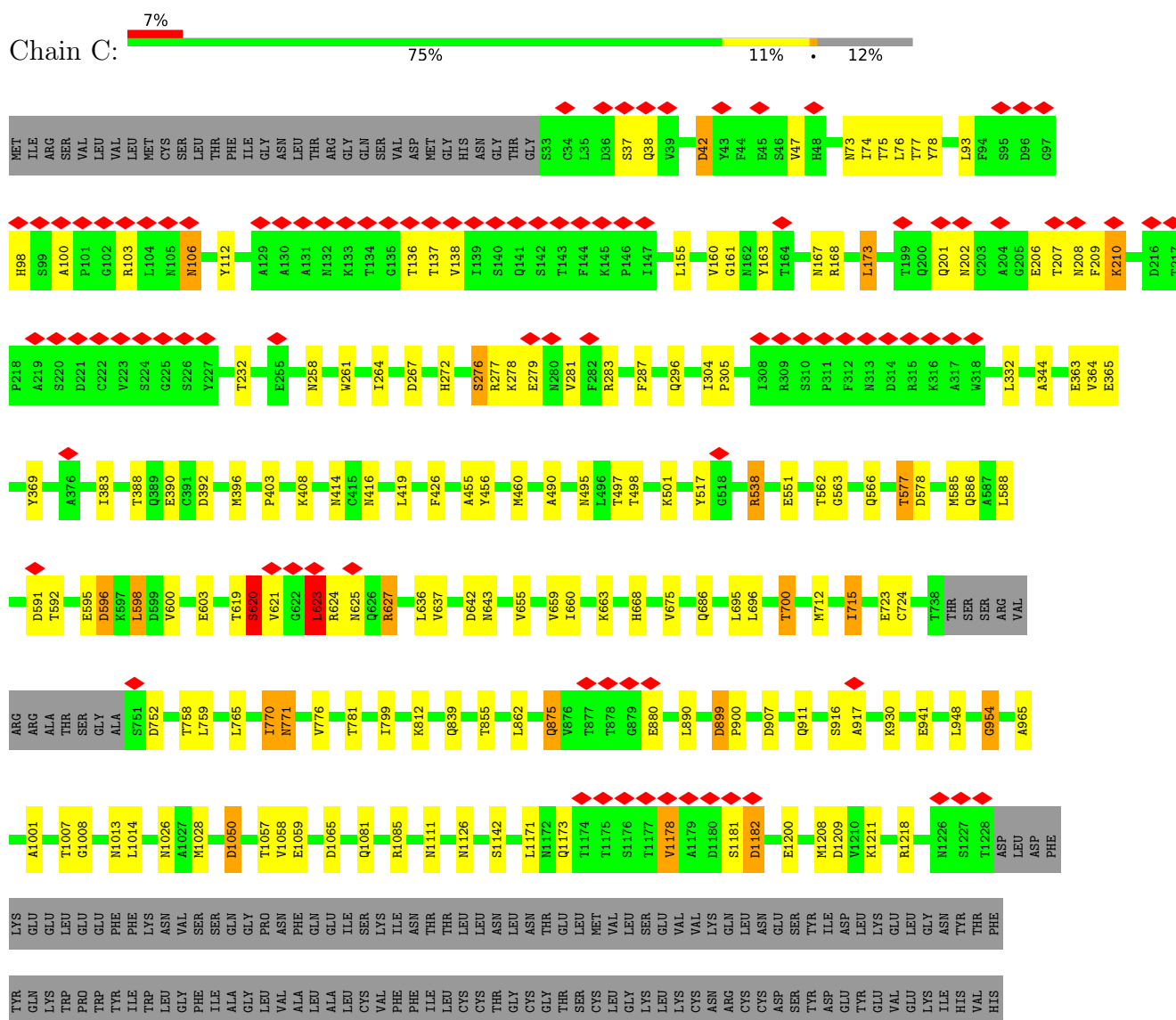
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5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

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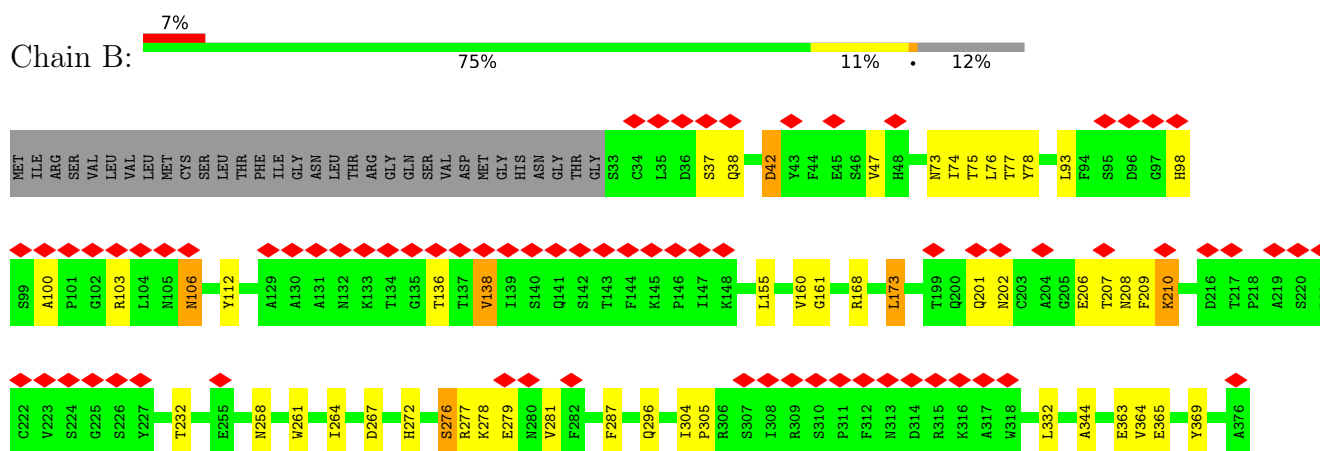
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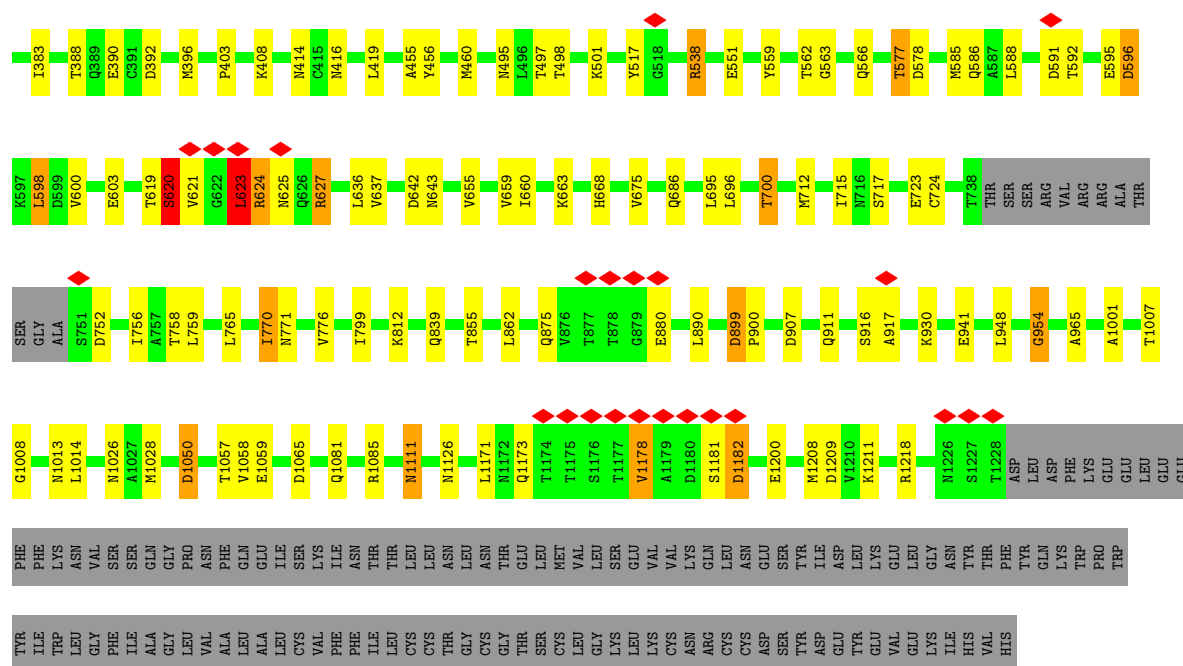
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5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

- Molecule 1: Spike glycoprotein



- Molecule 1: 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





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

Chain I:



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

Chain J:



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

Chain K:



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

Chain L:



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

Chain M:



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

Chain N:



- 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 Q:  50% 100%



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

Chain R:  100%



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

Chain S:  50% 50% 50%



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

Chain T:  50% 100%



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

Chain U:  50% 50% 50%



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



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



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



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



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



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





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



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



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



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



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(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, Not provided	
Number of particles used	40837	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	4.300	Depositor
Minimum map value	-2.491	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.135	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, 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	0.38	0/9413	0.63	5/12825 (0.0%)
1	B	0.38	0/9413	0.63	5/12825 (0.0%)
1	C	0.38	0/9413	0.63	5/12825 (0.0%)
All	All	0.38	0/28239	0.63	15/38475 (0.0%)

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	4
1	B	0	4
1	C	0	4
All	All	0	12

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	396	MET	N-CA-C	-5.93	107.28	114.75
1	B	396	MET	N-CA-C	-5.93	107.28	114.75
1	A	396	MET	N-CA-C	-5.92	107.29	114.75
1	A	1001	ALA	N-CA-C	-5.85	107.14	114.56
1	C	1001	ALA	N-CA-C	-5.83	107.16	114.56
1	B	1001	ALA	N-CA-C	-5.82	107.17	114.56
1	C	620	SER	CA-C-N	5.32	131.54	121.97
1	C	620	SER	C-N-CA	5.32	131.54	121.97
1	B	620	SER	CA-C-N	5.31	131.53	121.97
1	B	620	SER	C-N-CA	5.31	131.53	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	620	SER	CA-C-N	5.29	131.50	121.97
1	A	620	SER	C-N-CA	5.29	131.50	121.97
1	B	917	ALA	N-CA-C	-5.27	107.86	114.56
1	C	917	ALA	N-CA-C	-5.27	107.87	114.56
1	A	917	ALA	N-CA-C	-5.26	107.89	114.56

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	LEU	Peptide
1	A	625	ASN	Peptide
1	A	700	THR	Peptide
1	A	954	GLY	Peptide
1	B	623	LEU	Peptide
1	B	625	ASN	Peptide
1	B	700	THR	Peptide
1	B	954	GLY	Peptide
1	C	623	LEU	Peptide
1	C	625	ASN	Peptide
1	C	700	THR	Peptide
1	C	954	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9193	0	8838	65	0
1	B	9193	0	8838	57	0
1	C	9193	0	8838	61	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	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	0	0
2	W	28	0	25	0	0
2	X	28	0	25	0	0
2	Z	28	0	25	0	0
2	a	28	0	25	0	0
2	b	28	0	25	0	0
2	c	28	0	25	0	0
2	d	28	0	25	0	0
3	G	42	0	37	2	0
3	P	42	0	37	2	0
3	Y	42	0	37	2	0
4	A	18	0	31	2	0
4	B	18	0	31	3	0
4	C	18	0	31	2	0
5	A	140	0	130	1	0
5	B	140	0	130	1	0
5	C	140	0	130	1	0
All	All	28851	0	27708	186	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 3.

All (186) 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:655:VAL:H	1:C:686:GLN:HE22	1.47	0.62
1:A:655:VAL:H	1:A:686:GLN:HE22	1.47	0.62
1:B:655:VAL:H	1:B:686:GLN:HE22	1.47	0.62
1:B:724:CYS:HB2	1:B:759:LEU:HD21	1.83	0.60
1:A:724:CYS:HB2	1:A:759:LEU:HD21	1.83	0.60
1:C:724:CYS:HB2	1:C:759:LEU:HD21	1.83	0.59
1:C:106:ASN:N	1:C:106:ASN:OD1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LYS:HG3	1:B:279:GLU:HG3	1.85	0.58
1:B:100:ALA:HB3	1:B:103:ARG:HB2	1.85	0.58
1:B:112:TYR:HB2	1:B:305:PRO:HG3	1.86	0.58
1:A:106:ASN:N	1:A:106:ASN:OD1	2.37	0.58
1:C:112:TYR:HB2	1:C:305:PRO:HG3	1.85	0.58
1:C:100:ALA:HB3	1:C:103:ARG:HB2	1.85	0.58
1:A:112:TYR:HB2	1:A:305:PRO:HG3	1.85	0.57
1:B:106:ASN:OD1	1:B:106:ASN:N	2.37	0.57
1:A:278:LYS:HG3	1:A:279:GLU:HG3	1.85	0.57
1:C:627:ARG:NH2	1:C:642:ASP:OD1	2.38	0.57
1:B:1209:ASP:OD2	1:B:1211:LYS:NZ	2.36	0.57
1:C:278:LYS:HG3	1:C:279:GLU:HG3	1.85	0.57
1:C:596:ASP:OD1	1:C:596:ASP:N	2.37	0.57
1:B:168:ARG:NH1	1:B:209:PHE:O	2.38	0.57
1:A:100:ALA:HB3	1:A:103:ARG:HB2	1.85	0.56
1:C:168:ARG:NH1	1:C:209:PHE:O	2.38	0.56
1:A:627:ARG:NH2	1:A:642:ASP:OD1	2.38	0.56
1:B:1026:ASN:OD1	1:B:1085:ARG:NH2	2.38	0.56
1:A:168:ARG:NH1	1:A:209:PHE:O	2.38	0.56
1:A:596:ASP:N	1:A:596:ASP:OD1	2.37	0.56
1:A:577:THR:OG1	1:A:578:ASP:N	2.39	0.56
1:C:1026:ASN:OD1	1:C:1085:ARG:NH2	2.38	0.56
1:A:1209:ASP:OD2	1:A:1211:LYS:NZ	2.36	0.55
1:C:1209:ASP:OD2	1:C:1211:LYS:NZ	2.35	0.55
1:B:627:ARG:NH2	1:B:642:ASP:OD1	2.38	0.55
1:A:1026:ASN:OD1	1:A:1085:ARG:NH2	2.38	0.55
1:B:38:GLN:OE1	1:B:98:HIS:NE2	2.40	0.55
1:B:577:THR:OG1	1:B:578:ASP:N	2.39	0.55
1:C:261:TRP:H	1:C:276:SER:HB3	1.72	0.55
1:A:38:GLN:OE1	1:A:98:HIS:NE2	2.40	0.55
1:B:596:ASP:OD1	1:B:596:ASP:N	2.38	0.55
1:A:261:TRP:H	1:A:276:SER:HB3	1.72	0.54
1:C:38:GLN:OE1	1:C:98:HIS:NE2	2.40	0.54
1:A:416:ASN:HB3	1:A:585:MET:HG2	1.90	0.53
1:B:416:ASN:HB3	1:B:585:MET:HG2	1.90	0.53
1:B:261:TRP:H	1:B:276:SER:HB3	1.72	0.53
1:C:577:THR:OG1	1:C:578:ASP:N	2.39	0.53
1:B:455:ALA:HB3	4:B:3001:PLM:H61	1.91	0.53
1:A:37:SER:O	1:A:210:LYS:NZ	2.42	0.52
1:C:267:ASP:OD1	1:C:272:HIS:NE2	2.40	0.52
1:B:37:SER:O	1:B:210:LYS:NZ	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:SER:O	1:C:210:LYS:NZ	2.42	0.52
1:C:73:ASN:HD22	1:C:916:SER:HB3	1.75	0.52
1:C:416:ASN:HB3	1:C:585:MET:HG2	1.90	0.52
1:C:591:ASP:N	1:C:591:ASP:OD1	2.43	0.52
1:A:455:ALA:HB3	4:A:3001:PLM:H61	1.91	0.52
1:B:591:ASP:OD1	1:B:591:ASP:N	2.43	0.52
1:A:752:ASP:OD1	1:A:752:ASP:N	2.43	0.51
1:C:278:LYS:HB3	1:C:287:PHE:HB2	1.92	0.51
1:C:781:THR:HG1	1:C:1142:SER:HG	1.56	0.51
1:C:455:ALA:HB3	4:C:3001:PLM:H61	1.91	0.51
1:C:752:ASP:OD1	1:C:752:ASP:N	2.43	0.51
1:C:880:GLU:HA	3:G:3:NAG:H81	1.93	0.51
1:B:880:GLU:HA	3:P:3:NAG:H81	1.93	0.51
1:A:73:ASN:HD22	1:A:916:SER:HB3	1.75	0.51
1:A:591:ASP:N	1:A:591:ASP:OD1	2.43	0.51
1:A:880:GLU:HA	3:Y:3:NAG:H81	1.94	0.50
1:B:73:ASN:HD22	1:B:916:SER:HB3	1.75	0.50
1:C:1181:SER:O	1:C:1218:ARG:NH2	2.44	0.50
1:B:752:ASP:N	1:B:752:ASP:OD1	2.43	0.50
1:A:278:LYS:HB3	1:A:287:PHE:HB2	1.92	0.50
1:B:1181:SER:O	1:B:1218:ARG:NH2	2.44	0.50
1:B:278:LYS:HB3	1:B:287:PHE:HB2	1.92	0.50
1:A:267:ASP:OD1	1:A:272:HIS:NE2	2.40	0.49
1:B:267:ASP:OD1	1:B:272:HIS:NE2	2.40	0.49
1:A:201:GLN:NE2	1:A:202:ASN:OD1	2.46	0.49
1:B:954:GLY:HA2	1:B:965:ALA:H	1.78	0.49
1:A:1181:SER:O	1:A:1218:ARG:NH2	2.44	0.49
1:A:403:PRO:HB3	4:A:3001:PLM:H72	1.95	0.49
1:B:201:GLN:NE2	1:B:202:ASN:OD1	2.46	0.49
1:A:1008:GLY:O	1:A:1013:ASN:ND2	2.45	0.49
1:B:403:PRO:HB3	4:B:3001:PLM:H72	1.95	0.49
1:A:456:TYR:OH	1:A:460:MET:O	2.30	0.48
1:C:1008:GLY:O	1:C:1013:ASN:ND2	2.45	0.48
1:B:1050:ASP:N	1:B:1050:ASP:OD1	2.46	0.48
1:C:954:GLY:HA2	1:C:965:ALA:H	1.78	0.48
1:A:1050:ASP:N	1:A:1050:ASP:OD1	2.46	0.48
1:A:954:GLY:HA2	1:A:965:ALA:H	1.78	0.48
1:B:1008:GLY:O	1:B:1013:ASN:ND2	2.45	0.48
1:C:201:GLN:NE2	1:C:202:ASN:OD1	2.46	0.48
1:A:42:ASP:N	1:A:42:ASP:OD1	2.46	0.48
1:B:332:LEU:O	1:B:344:ALA:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:O	1:A:344:ALA:HA	2.14	0.48
1:A:365:GLU:O	1:A:369:TYR:OH	2.32	0.47
1:C:1050:ASP:N	1:C:1050:ASP:OD1	2.46	0.47
1:A:1208:MET:HE3	1:A:1208:MET:HB3	1.84	0.47
1:C:42:ASP:N	1:C:42:ASP:OD1	2.46	0.47
1:B:456:TYR:OH	1:B:460:MET:O	2.30	0.47
1:C:501:LYS:NZ	1:C:563:GLY:O	2.48	0.47
1:B:42:ASP:OD1	1:B:42:ASP:N	2.46	0.47
1:B:365:GLU:O	1:B:369:TYR:OH	2.33	0.47
1:B:501:LYS:NZ	1:B:563:GLY:O	2.48	0.47
1:C:403:PRO:HB3	4:C:3001:PLM:H72	1.95	0.47
1:B:1111:ASN:OD1	1:B:1111:ASN:N	2.39	0.47
1:C:332:LEU:O	1:C:344:ALA:HA	2.14	0.46
1:A:655:VAL:HG13	1:A:675:VAL:HG21	1.97	0.46
1:B:161:GLY:HA3	1:B:173:LEU:HD21	1.97	0.46
1:B:365:GLU:OE1	1:B:663:LYS:NZ	2.46	0.46
1:A:161:GLY:HA3	1:A:173:LEU:HD21	1.97	0.46
1:C:365:GLU:O	1:C:369:TYR:OH	2.33	0.46
1:C:655:VAL:HG13	1:C:675:VAL:HG21	1.97	0.46
1:C:538:ARG:H	1:C:538:ARG:HG2	1.44	0.46
1:C:161:GLY:HA3	1:C:173:LEU:HD21	1.97	0.46
1:A:501:LYS:NZ	1:A:563:GLY:O	2.48	0.46
1:C:456:TYR:OH	1:C:460:MET:O	2.30	0.46
1:C:941:GLU:O	1:C:1126:ASN:ND2	2.46	0.46
1:B:277:ARG:HG2	1:B:281:VAL:HG23	1.98	0.46
1:C:277:ARG:HG2	1:C:281:VAL:HG23	1.98	0.45
1:A:277:ARG:HG2	1:A:281:VAL:HG23	1.98	0.45
1:A:365:GLU:OE1	1:A:663:LYS:NZ	2.46	0.45
1:B:770:ILE:H	1:B:770:ILE:HG13	1.62	0.45
1:B:655:VAL:HG13	1:B:675:VAL:HG21	1.97	0.45
1:C:408:LYS:HE3	1:C:408:LYS:HB2	1.79	0.45
1:C:770:ILE:H	1:C:770:ILE:HG13	1.62	0.45
1:A:1111:ASN:OD1	1:A:1111:ASN:N	2.39	0.45
1:B:538:ARG:H	1:B:538:ARG:HG2	1.44	0.45
1:A:408:LYS:HE3	1:A:408:LYS:HB2	1.79	0.45
1:A:941:GLU:O	1:A:1126:ASN:ND2	2.46	0.45
1:B:408:LYS:HE3	1:B:408:LYS:HB2	1.79	0.45
1:A:538:ARG:H	1:A:538:ARG:HG2	1.44	0.44
1:A:771:ASN:OD1	1:A:771:ASN:N	2.48	0.44
1:C:620:SER:HB3	1:C:621:VAL:H	1.49	0.44
1:A:620:SER:HB3	1:A:621:VAL:H	1.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1178:VAL:HG12	1:C:1182:ASP:HB2	1.99	0.44
1:C:365:GLU:OE1	1:C:663:LYS:NZ	2.46	0.44
1:C:660:ILE:O	1:C:668:HIS:HA	2.17	0.44
1:A:660:ILE:O	1:A:668:HIS:HA	2.17	0.44
1:B:559:TYR:OH	4:B:3001:PLM:O2	2.29	0.44
1:C:155:LEU:HD13	1:C:304:ILE:HD11	2.00	0.44
1:C:715:ILE:HD13	1:C:715:ILE:HA	1.88	0.44
1:B:660:ILE:O	1:B:668:HIS:HA	2.17	0.43
1:B:155:LEU:HD13	1:B:304:ILE:HD11	2.00	0.43
1:C:598:LEU:HD12	5:C:3009:NAG:H61	2.01	0.43
1:C:771:ASN:OD1	1:C:771:ASN:N	2.48	0.43
3:G:1:NAG:H61	3:G:2:NAG:HN2	1.84	0.43
3:Y:1:NAG:H61	3:Y:2:NAG:HN2	1.84	0.43
1:A:366:THR:HG1	1:A:663:LYS:H	1.66	0.43
1:A:598:LEU:HD12	5:A:3009:NAG:H61	2.01	0.43
1:A:1173:GLN:H	1:A:1173:GLN:HG3	1.54	0.43
1:A:155:LEU:HD13	1:A:304:ILE:HD11	2.00	0.43
1:B:941:GLU:O	1:B:1126:ASN:ND2	2.45	0.43
1:C:712:MET:HB3	1:C:712:MET:HE2	1.81	0.43
1:B:717:SER:OG	1:B:756:ILE:O	2.31	0.43
3:P:1:NAG:H61	3:P:2:NAG:HN2	1.84	0.43
1:A:149:LYS:NZ	1:A:256:ASP:O	2.49	0.43
1:C:283:ARG:HA	1:C:283:ARG:HD2	1.79	0.43
1:A:1178:VAL:HG12	1:A:1182:ASP:HB2	1.99	0.43
1:C:875:GLN:H	1:C:875:GLN:HG2	1.65	0.43
1:B:598:LEU:HD12	5:B:3009:NAG:H61	2.01	0.43
1:C:383:ILE:H	1:C:592:THR:HB	1.84	0.42
1:B:1178:VAL:HG12	1:B:1182:ASP:HB2	1.99	0.42
1:A:899:ASP:HA	1:A:900:PRO:HD3	1.88	0.42
1:B:206:GLU:HB3	1:B:208:ASN:H	1.84	0.42
1:A:163:TYR:O	1:A:167:ASN:N	2.51	0.42
1:A:383:ILE:H	1:A:592:THR:HB	1.84	0.42
1:C:206:GLU:HB3	1:C:208:ASN:H	1.84	0.42
1:B:383:ILE:H	1:B:592:THR:HB	1.84	0.42
1:B:712:MET:HE2	1:B:712:MET:HB3	1.81	0.42
1:A:717:SER:OG	1:A:756:ILE:O	2.31	0.42
1:A:206:GLU:HB3	1:A:208:ASN:H	1.84	0.42
1:B:620:SER:HB3	1:B:621:VAL:H	1.49	0.42
1:B:624:ARG:HA	1:B:624:ARG:HD2	1.58	0.42
1:A:174:ASN:HD22	1:A:174:ASN:HA	1.53	0.41
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:THR:O	1:C:137:THR:OG1	2.32	0.41
1:C:598:LEU:HD23	1:C:598:LEU:HA	1.89	0.41
1:C:163:TYR:O	1:C:167:ASN:N	2.51	0.41
1:A:770:ILE:H	1:A:770:ILE:HG13	1.62	0.41
1:B:1208:MET:HB3	1:B:1208:MET:HE3	1.84	0.41
1:C:899:ASP:HA	1:C:900:PRO:HD3	1.88	0.41
1:C:1208:MET:HE3	1:C:1208:MET:HB3	1.84	0.41
1:A:283:ARG:HD2	1:A:283:ARG:HA	1.79	0.41
1:A:426:PHE:HB3	1:A:490:ALA:HB1	2.03	0.41
1:C:426:PHE:HB3	1:C:490:ALA:HB1	2.03	0.41
1:B:899:ASP:HA	1:B:900:PRO:HD3	1.87	0.41
1:A:148:LYS:N	1:A:317:ALA:O	2.50	0.40
1:B:138:VAL:H	1:B:138:VAL:HG23	1.63	0.40
1:A:1075:LEU:HD23	1:A:1075:LEU:HA	1.93	0.40
1:A:875:GLN:H	1:A:875:GLN:HG2	1.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1180/1352 (87%)	1109 (94%)	70 (6%)	1 (0%)	48	77
1	B	1180/1352 (87%)	1110 (94%)	69 (6%)	1 (0%)	48	77
1	C	1180/1352 (87%)	1108 (94%)	71 (6%)	1 (0%)	48	77
All	All	3540/4056 (87%)	3327 (94%)	210 (6%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	623	LEU
1	C	623	LEU

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Mol	Chain	Res	Type
1	B	623	LEU

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	1022/1172 (87%)	933 (91%)	89 (9%)	8	26
1	B	1022/1172 (87%)	933 (91%)	89 (9%)	8	26
1	C	1022/1172 (87%)	933 (91%)	89 (9%)	8	26
All	All	3066/3516 (87%)	2799 (91%)	267 (9%)	11	26

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	47	VAL
1	A	74	ILE
1	A	75	THR
1	A	76	LEU
1	A	77	THR
1	A	78	TYR
1	A	93	LEU
1	A	106	ASN
1	A	136	THR
1	A	138	VAL
1	A	160	VAL
1	A	173	LEU
1	A	207	THR
1	A	210	LYS
1	A	232	THR
1	A	258	ASN
1	A	264	ILE
1	A	276	SER
1	A	296	GLN
1	A	363	GLU

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Mol	Chain	Res	Type
1	A	364	VAL
1	A	388	THR
1	A	390	GLU
1	A	392	ASP
1	A	414	ASN
1	A	419	LEU
1	A	495	ASN
1	A	497	THR
1	A	498	THR
1	A	517	TYR
1	A	538	ARG
1	A	551	GLU
1	A	562	THR
1	A	566	GLN
1	A	577	THR
1	A	586	GLN
1	A	588	LEU
1	A	595	GLU
1	A	596	ASP
1	A	598	LEU
1	A	600	VAL
1	A	603	GLU
1	A	619	THR
1	A	620	SER
1	A	623	LEU
1	A	624	ARG
1	A	627	ARG
1	A	636	LEU
1	A	637	VAL
1	A	643	ASN
1	A	659	VAL
1	A	695	LEU
1	A	696	LEU
1	A	700	THR
1	A	715	ILE
1	A	723	GLU
1	A	758	THR
1	A	765	LEU
1	A	770	ILE
1	A	771	ASN
1	A	776	VAL
1	A	799	ILE

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Mol	Chain	Res	Type
1	A	812	LYS
1	A	839	GLN
1	A	855	THR
1	A	862	LEU
1	A	875	GLN
1	A	890	LEU
1	A	899	ASP
1	A	907	ASP
1	A	911	GLN
1	A	930	LYS
1	A	948	LEU
1	A	1007	THR
1	A	1014	LEU
1	A	1028	MET
1	A	1050	ASP
1	A	1057	THR
1	A	1058	VAL
1	A	1059	GLU
1	A	1065	ASP
1	A	1081	GLN
1	A	1111	ASN
1	A	1171	LEU
1	A	1173	GLN
1	A	1178	VAL
1	A	1182	ASP
1	A	1200	GLU
1	C	42	ASP
1	C	47	VAL
1	C	74	ILE
1	C	75	THR
1	C	76	LEU
1	C	77	THR
1	C	78	TYR
1	C	93	LEU
1	C	106	ASN
1	C	136	THR
1	C	138	VAL
1	C	160	VAL
1	C	173	LEU
1	C	207	THR
1	C	210	LYS
1	C	232	THR

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Mol	Chain	Res	Type
1	C	258	ASN
1	C	264	ILE
1	C	276	SER
1	C	296	GLN
1	C	363	GLU
1	C	364	VAL
1	C	388	THR
1	C	390	GLU
1	C	392	ASP
1	C	414	ASN
1	C	419	LEU
1	C	495	ASN
1	C	497	THR
1	C	498	THR
1	C	517	TYR
1	C	538	ARG
1	C	551	GLU
1	C	562	THR
1	C	566	GLN
1	C	577	THR
1	C	586	GLN
1	C	588	LEU
1	C	595	GLU
1	C	596	ASP
1	C	598	LEU
1	C	600	VAL
1	C	603	GLU
1	C	619	THR
1	C	620	SER
1	C	623	LEU
1	C	624	ARG
1	C	627	ARG
1	C	636	LEU
1	C	637	VAL
1	C	643	ASN
1	C	659	VAL
1	C	695	LEU
1	C	696	LEU
1	C	700	THR
1	C	715	ILE
1	C	723	GLU
1	C	758	THR

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Mol	Chain	Res	Type
1	C	765	LEU
1	C	770	ILE
1	C	771	ASN
1	C	776	VAL
1	C	799	ILE
1	C	812	LYS
1	C	839	GLN
1	C	855	THR
1	C	862	LEU
1	C	875	GLN
1	C	890	LEU
1	C	899	ASP
1	C	907	ASP
1	C	911	GLN
1	C	930	LYS
1	C	948	LEU
1	C	1007	THR
1	C	1014	LEU
1	C	1028	MET
1	C	1050	ASP
1	C	1057	THR
1	C	1058	VAL
1	C	1059	GLU
1	C	1065	ASP
1	C	1081	GLN
1	C	1111	ASN
1	C	1171	LEU
1	C	1173	GLN
1	C	1178	VAL
1	C	1182	ASP
1	C	1200	GLU
1	B	42	ASP
1	B	47	VAL
1	B	74	ILE
1	B	75	THR
1	B	76	LEU
1	B	77	THR
1	B	78	TYR
1	B	93	LEU
1	B	106	ASN
1	B	136	THR
1	B	138	VAL

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Mol	Chain	Res	Type
1	B	160	VAL
1	B	173	LEU
1	B	207	THR
1	B	210	LYS
1	B	232	THR
1	B	258	ASN
1	B	264	ILE
1	B	276	SER
1	B	296	GLN
1	B	363	GLU
1	B	364	VAL
1	B	388	THR
1	B	390	GLU
1	B	392	ASP
1	B	414	ASN
1	B	419	LEU
1	B	495	ASN
1	B	497	THR
1	B	498	THR
1	B	517	TYR
1	B	538	ARG
1	B	551	GLU
1	B	562	THR
1	B	566	GLN
1	B	577	THR
1	B	586	GLN
1	B	588	LEU
1	B	595	GLU
1	B	596	ASP
1	B	598	LEU
1	B	600	VAL
1	B	603	GLU
1	B	619	THR
1	B	620	SER
1	B	623	LEU
1	B	624	ARG
1	B	627	ARG
1	B	636	LEU
1	B	637	VAL
1	B	643	ASN
1	B	659	VAL
1	B	695	LEU

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Mol	Chain	Res	Type
1	B	696	LEU
1	B	700	THR
1	B	715	ILE
1	B	723	GLU
1	B	758	THR
1	B	765	LEU
1	B	770	ILE
1	B	771	ASN
1	B	776	VAL
1	B	799	ILE
1	B	812	LYS
1	B	839	GLN
1	B	855	THR
1	B	862	LEU
1	B	875	GLN
1	B	890	LEU
1	B	899	ASP
1	B	907	ASP
1	B	911	GLN
1	B	930	LYS
1	B	948	LEU
1	B	1007	THR
1	B	1014	LEU
1	B	1028	MET
1	B	1050	ASP
1	B	1057	THR
1	B	1058	VAL
1	B	1059	GLU
1	B	1065	ASP
1	B	1081	GLN
1	B	1111	ASN
1	B	1171	LEU
1	B	1173	GLN
1	B	1178	VAL
1	B	1182	ASP
1	B	1200	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	91	GLN

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Mol	Chain	Res	Type
1	A	158	HIS
1	A	201	GLN
1	A	202	ASN
1	A	208	ASN
1	A	416	ASN
1	A	645	ASN
1	A	686	GLN
1	A	755	GLN
1	A	823	GLN
1	A	859	GLN
1	A	875	GLN
1	A	904	GLN
1	A	971	GLN
1	A	1020	GLN
1	A	1097	GLN
1	A	1173	GLN
1	C	91	GLN
1	C	158	HIS
1	C	201	GLN
1	C	202	ASN
1	C	208	ASN
1	C	416	ASN
1	C	645	ASN
1	C	686	GLN
1	C	755	GLN
1	C	809	ASN
1	C	823	GLN
1	C	859	GLN
1	C	875	GLN
1	C	904	GLN
1	C	971	GLN
1	C	1020	GLN
1	C	1097	GLN
1	C	1173	GLN
1	B	91	GLN
1	B	158	HIS
1	B	208	ASN
1	B	416	ASN
1	B	645	ASN
1	B	686	GLN
1	B	755	GLN
1	B	809	ASN

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Mol	Chain	Res	Type
1	B	823	GLN
1	B	859	GLN
1	B	875	GLN
1	B	904	GLN
1	B	924	GLN
1	B	971	GLN
1	B	1020	GLN
1	B	1097	GLN
1	B	1173	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

57 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	0.48	0	17,19,21	0.65	0
2	NAG	D	2	2	14,14,15	0.33	0	17,19,21	0.64	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.26	0	17,19,21	0.49	0
2	NAG	E	2	2	14,14,15	0.44	0	17,19,21	0.43	0
2	NAG	F	1	1,2	14,14,15	0.46	0	17,19,21	0.71	1 (5%)
2	NAG	F	2	2	14,14,15	0.31	0	17,19,21	0.48	0
3	NAG	G	1	1,3	14,14,15	0.62	1 (7%)	17,19,21	0.71	0
3	NAG	G	2	3	14,14,15	0.19	0	17,19,21	0.64	0
3	NAG	G	3	3	14,14,15	0.36	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	H	1	1,2	14,14,15	0.21	0	17,19,21	0.55	0
2	NAG	H	2	2	14,14,15	0.26	0	17,19,21	0.55	0
2	NAG	I	1	1,2	14,14,15	0.29	0	17,19,21	0.52	0
2	NAG	I	2	2	14,14,15	0.32	0	17,19,21	0.47	0
2	NAG	J	1	1,2	14,14,15	0.47	0	17,19,21	0.87	1 (5%)
2	NAG	J	2	2	14,14,15	0.43	0	17,19,21	0.53	0
2	NAG	K	1	1,2	14,14,15	0.33	0	17,19,21	0.50	0
2	NAG	K	2	2	14,14,15	0.29	0	17,19,21	0.50	0
2	NAG	L	1	1,2	14,14,15	0.29	0	17,19,21	0.62	0
2	NAG	L	2	2	14,14,15	0.22	0	17,19,21	0.60	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.47	0	17,19,21	0.66	0
2	NAG	M	2	2	14,14,15	0.32	0	17,19,21	0.63	1 (5%)
2	NAG	N	1	1,2	14,14,15	0.26	0	17,19,21	0.49	0
2	NAG	N	2	2	14,14,15	0.44	0	17,19,21	0.43	0
2	NAG	O	1	1,2	14,14,15	0.47	0	17,19,21	0.70	1 (5%)
2	NAG	O	2	2	14,14,15	0.31	0	17,19,21	0.48	0
3	NAG	P	1	1,3	14,14,15	0.61	1 (7%)	17,19,21	0.71	0
3	NAG	P	2	3	14,14,15	0.20	0	17,19,21	0.64	0
3	NAG	P	3	3	14,14,15	0.35	0	17,19,21	0.58	0
2	NAG	Q	1	1,2	14,14,15	0.20	0	17,19,21	0.54	0
2	NAG	Q	2	2	14,14,15	0.24	0	17,19,21	0.55	0
2	NAG	R	1	1,2	14,14,15	0.28	0	17,19,21	0.51	0
2	NAG	R	2	2	14,14,15	0.31	0	17,19,21	0.46	0
2	NAG	S	1	1,2	14,14,15	0.46	0	17,19,21	0.87	1 (5%)
2	NAG	S	2	2	14,14,15	0.42	0	17,19,21	0.53	0
2	NAG	T	1	1,2	14,14,15	0.34	0	17,19,21	0.51	0
2	NAG	T	2	2	14,14,15	0.29	0	17,19,21	0.51	0
2	NAG	U	1	1,2	14,14,15	0.28	0	17,19,21	0.63	0
2	NAG	U	2	2	14,14,15	0.22	0	17,19,21	0.59	1 (5%)
2	NAG	V	1	1,2	14,14,15	0.47	0	17,19,21	0.66	0
2	NAG	V	2	2	14,14,15	0.31	0	17,19,21	0.63	1 (5%)
2	NAG	W	1	1,2	14,14,15	0.27	0	17,19,21	0.49	0
2	NAG	W	2	2	14,14,15	0.45	0	17,19,21	0.44	0
2	NAG	X	1	1,2	14,14,15	0.45	0	17,19,21	0.70	1 (5%)
2	NAG	X	2	2	14,14,15	0.32	0	17,19,21	0.47	0
3	NAG	Y	1	1,3	14,14,15	0.62	1 (7%)	17,19,21	0.71	0
3	NAG	Y	2	3	14,14,15	0.21	0	17,19,21	0.63	0
3	NAG	Y	3	3	14,14,15	0.35	0	17,19,21	0.58	0
2	NAG	Z	1	1,2	14,14,15	0.21	0	17,19,21	0.54	0
2	NAG	Z	2	2	14,14,15	0.25	0	17,19,21	0.56	0
2	NAG	a	1	1,2	14,14,15	0.27	0	17,19,21	0.51	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	0.32	0	17,19,21	0.46	0
2	NAG	b	1	1,2	14,14,15	0.47	0	17,19,21	0.88	1 (5%)
2	NAG	b	2	2	14,14,15	0.43	0	17,19,21	0.53	0
2	NAG	c	1	1,2	14,14,15	0.34	0	17,19,21	0.50	0
2	NAG	c	2	2	14,14,15	0.30	0	17,19,21	0.50	0
2	NAG	d	1	1,2	14,14,15	0.28	0	17,19,21	0.62	0
2	NAG	d	2	2	14,14,15	0.22	0	17,19,21	0.59	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	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	3	3	-	1/6/23/26	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	-	2/6/23/26	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	-	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	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	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	-	0/6/23/26	0/1/1/1
2	NAG	O	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	O	2	2	-	0/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	3	3	-	1/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	2/6/23/26	0/1/1/1
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	-	2/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	2/6/23/26	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	-	2/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	2/6/23/26	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
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Y	3	3	-	1/6/23/26	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
2	NAG	b	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	b	2	2	-	2/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	c	2	2	-	2/6/23/26	0/1/1/1
2	NAG	d	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	d	2	2	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	1	NAG	O5-C1	-2.17	1.40	1.43
3	G	1	NAG	O5-C1	-2.17	1.40	1.43
3	P	1	NAG	O5-C1	-2.12	1.40	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	1	NAG	C1-O5-C5	2.75	115.92	112.19
2	J	1	NAG	C1-O5-C5	2.73	115.90	112.19
2	S	1	NAG	C1-O5-C5	2.73	115.89	112.19
2	F	1	NAG	C1-O5-C5	2.36	115.39	112.19
2	X	1	NAG	C1-O5-C5	2.34	115.36	112.19
2	O	1	NAG	C1-O5-C5	2.32	115.33	112.19
2	D	2	NAG	C1-O5-C5	2.25	115.24	112.19
2	M	2	NAG	C1-O5-C5	2.23	115.22	112.19
2	V	2	NAG	C1-O5-C5	2.22	115.19	112.19
2	L	2	NAG	C1-O5-C5	2.14	115.09	112.19
2	d	2	NAG	C1-O5-C5	2.10	115.03	112.19
2	U	2	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	1	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	d	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	V	1	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	d	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	b	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	b	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	a	1	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	Z	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
2	Z	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	V	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
3	G	3	NAG	O5-C5-C6-O6
3	P	3	NAG	O5-C5-C6-O6
3	Y	3	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	U	2	NAG	C4-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	b	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	c	2	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	c	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	a	2	NAG	C4-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 6 short contacts:

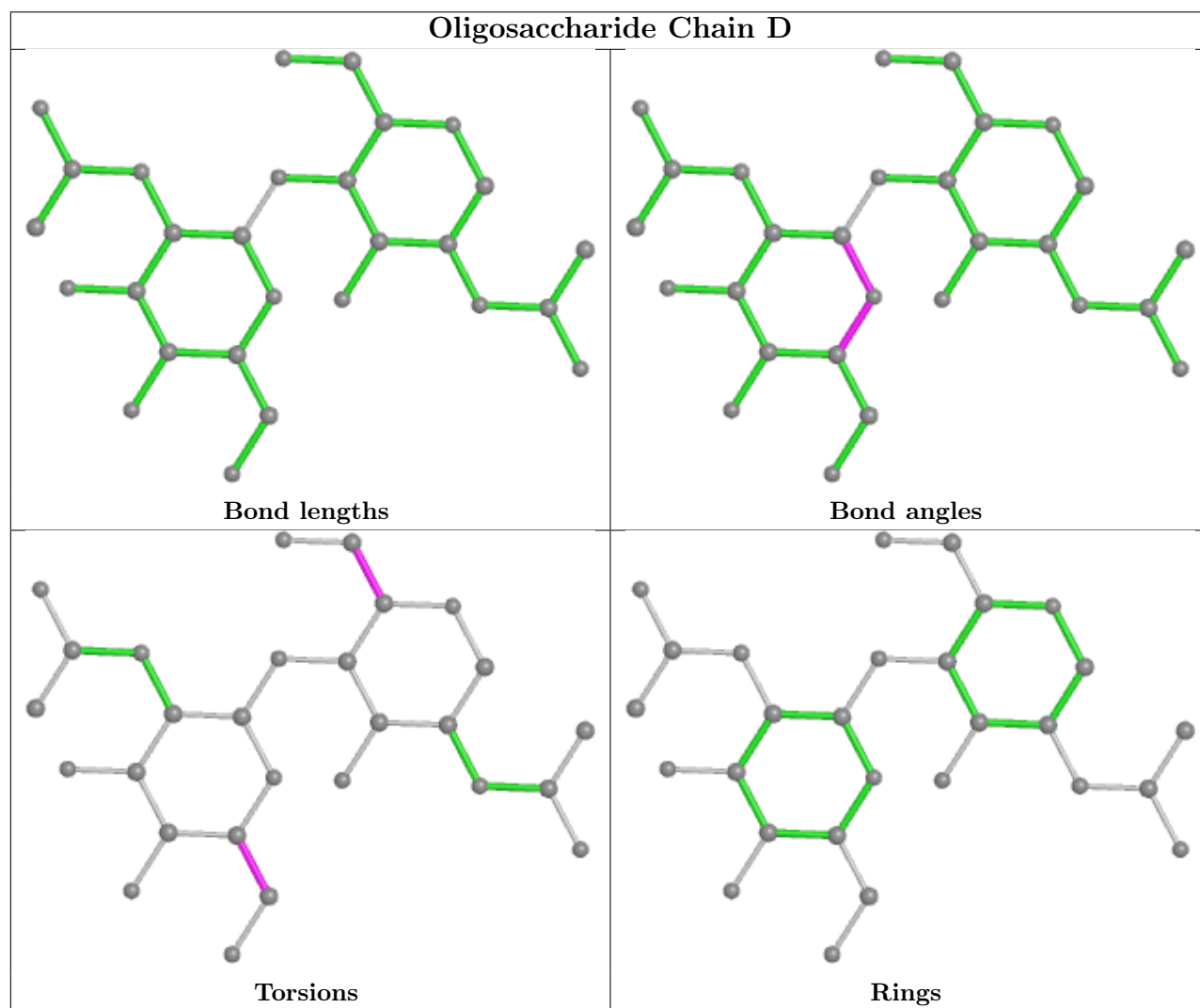
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
3	Y	1	NAG	1	0
3	P	1	NAG	1	0
3	P	2	NAG	1	0

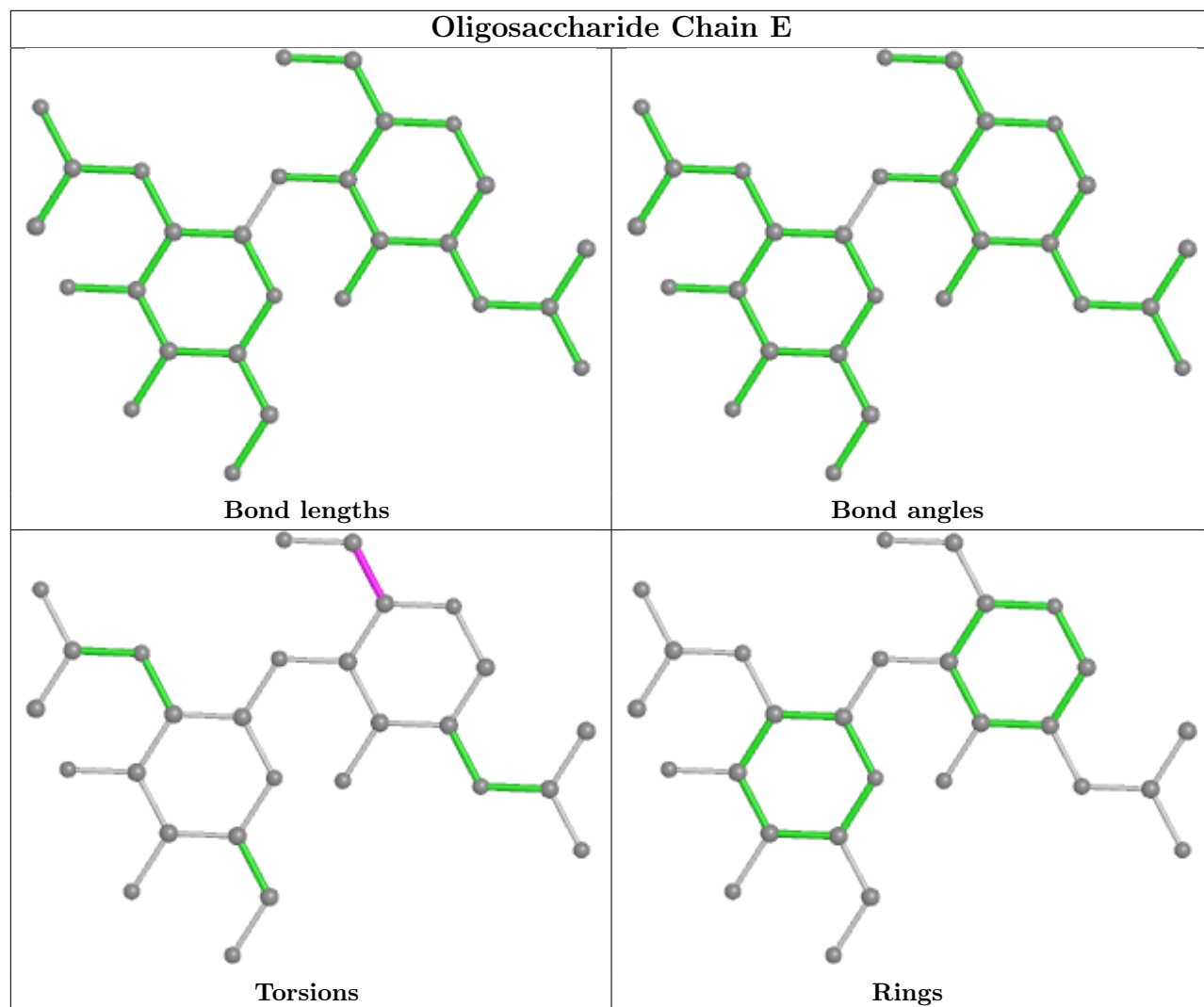
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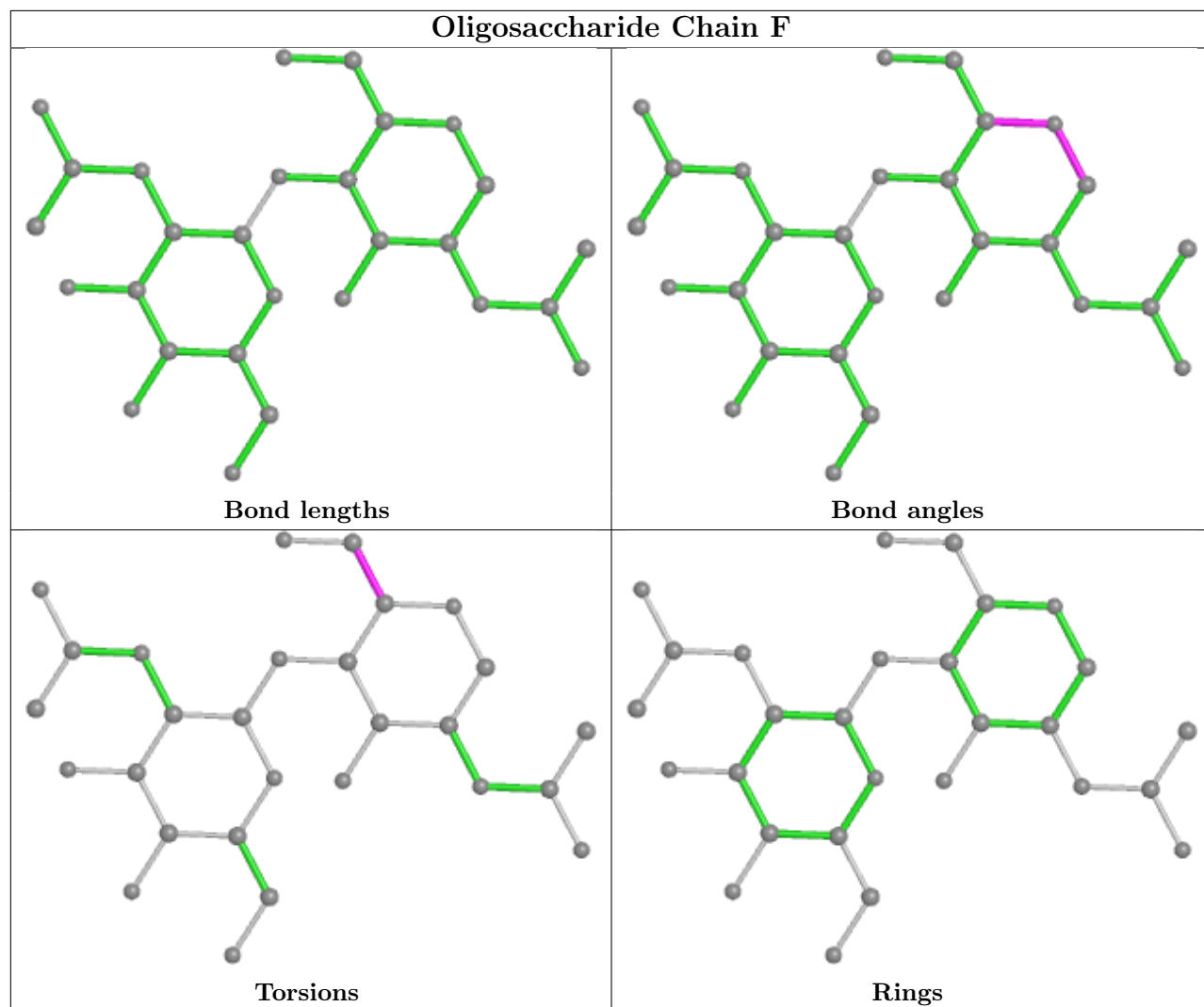
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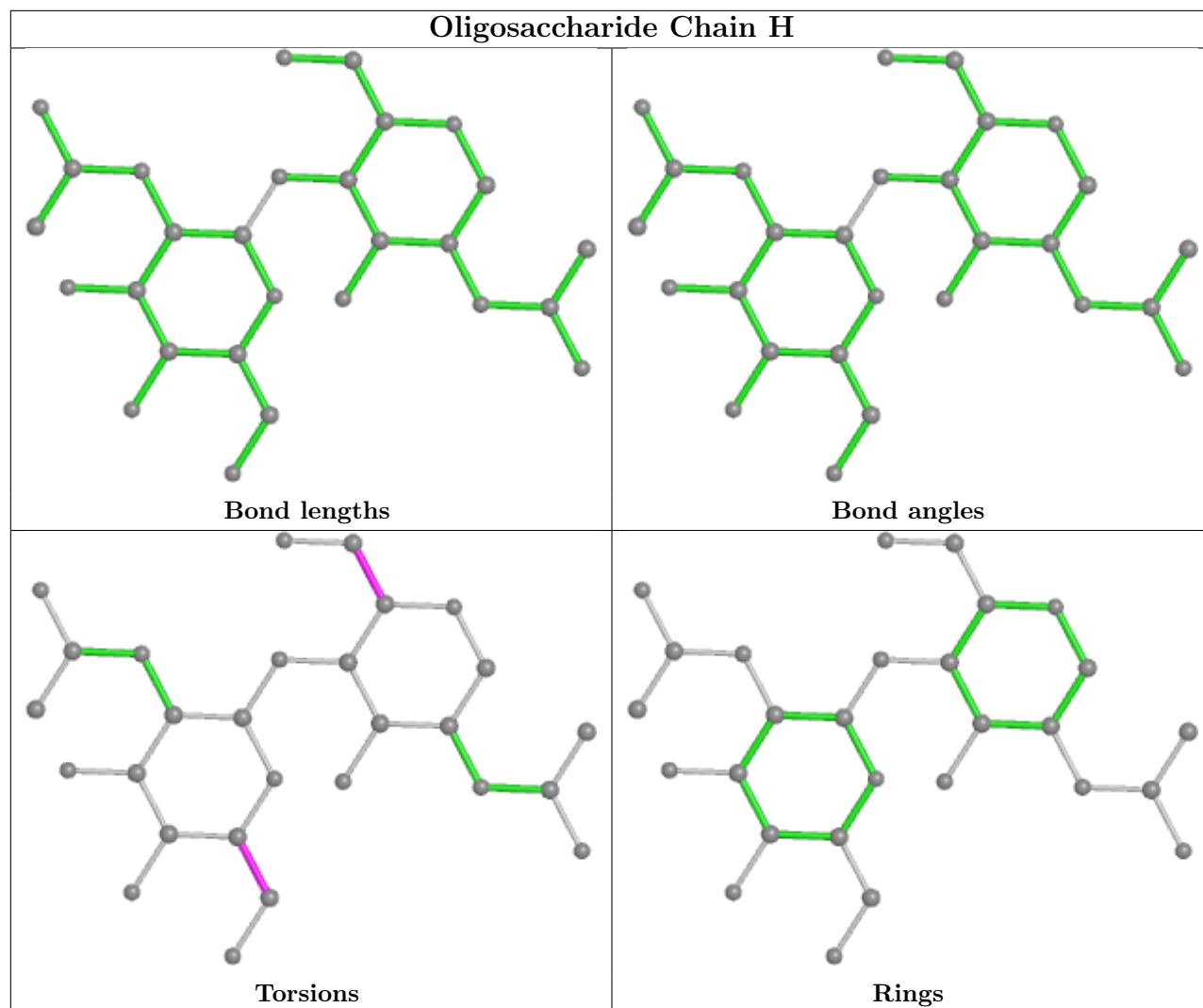
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	2	NAG	1	0
3	G	2	NAG	1	0
3	G	3	NAG	1	0
3	Y	3	NAG	1	0
3	P	3	NAG	1	0

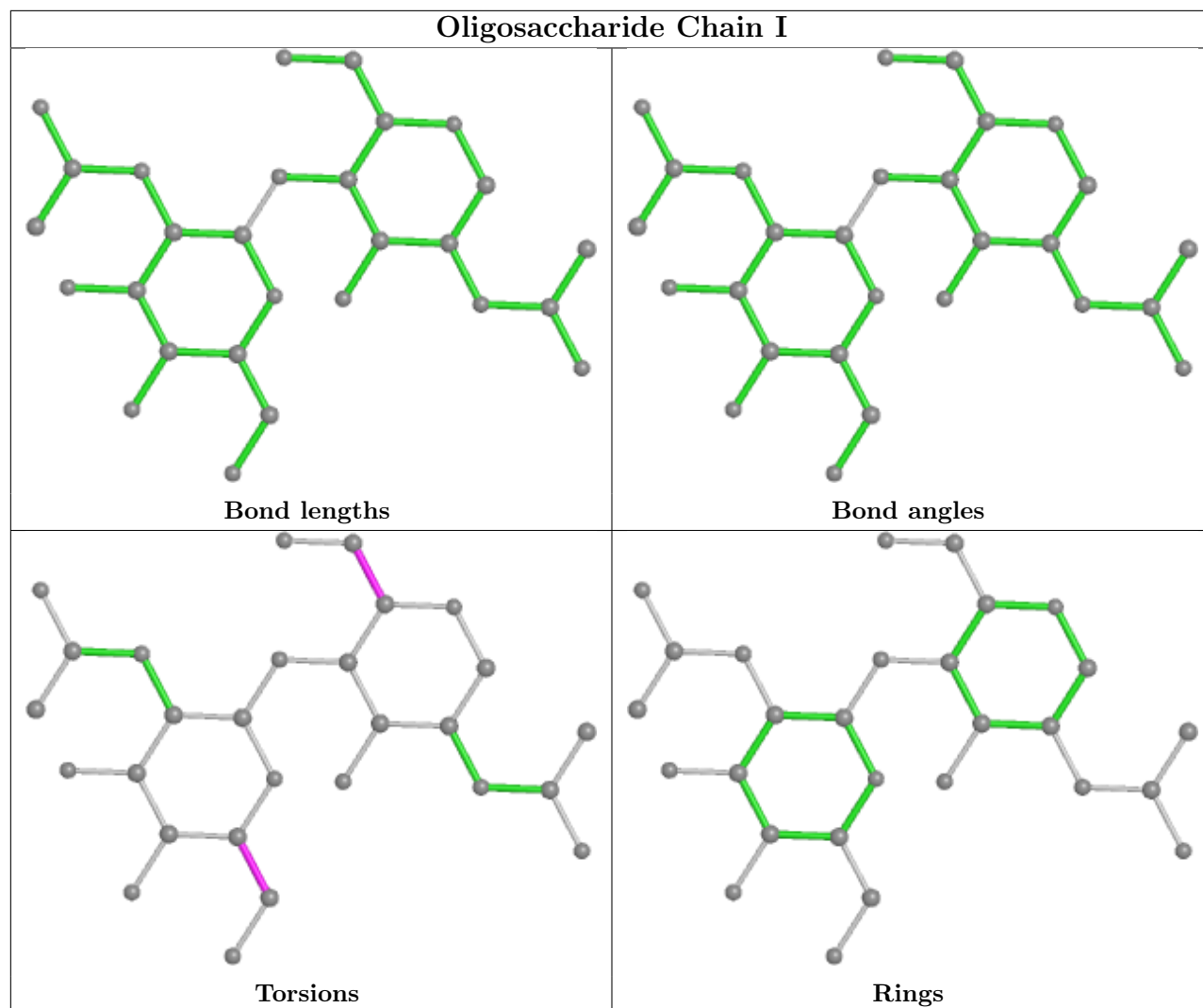
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

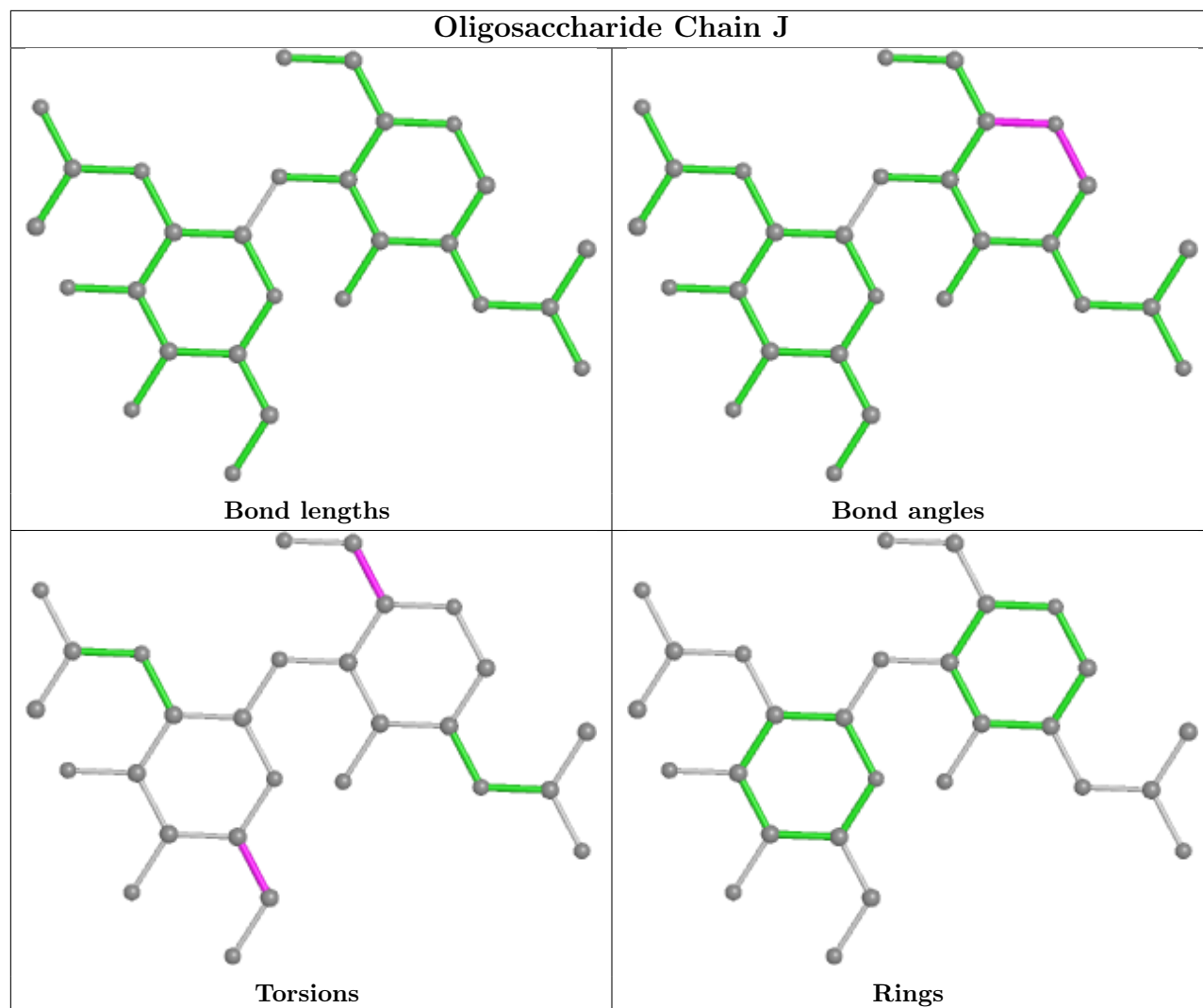


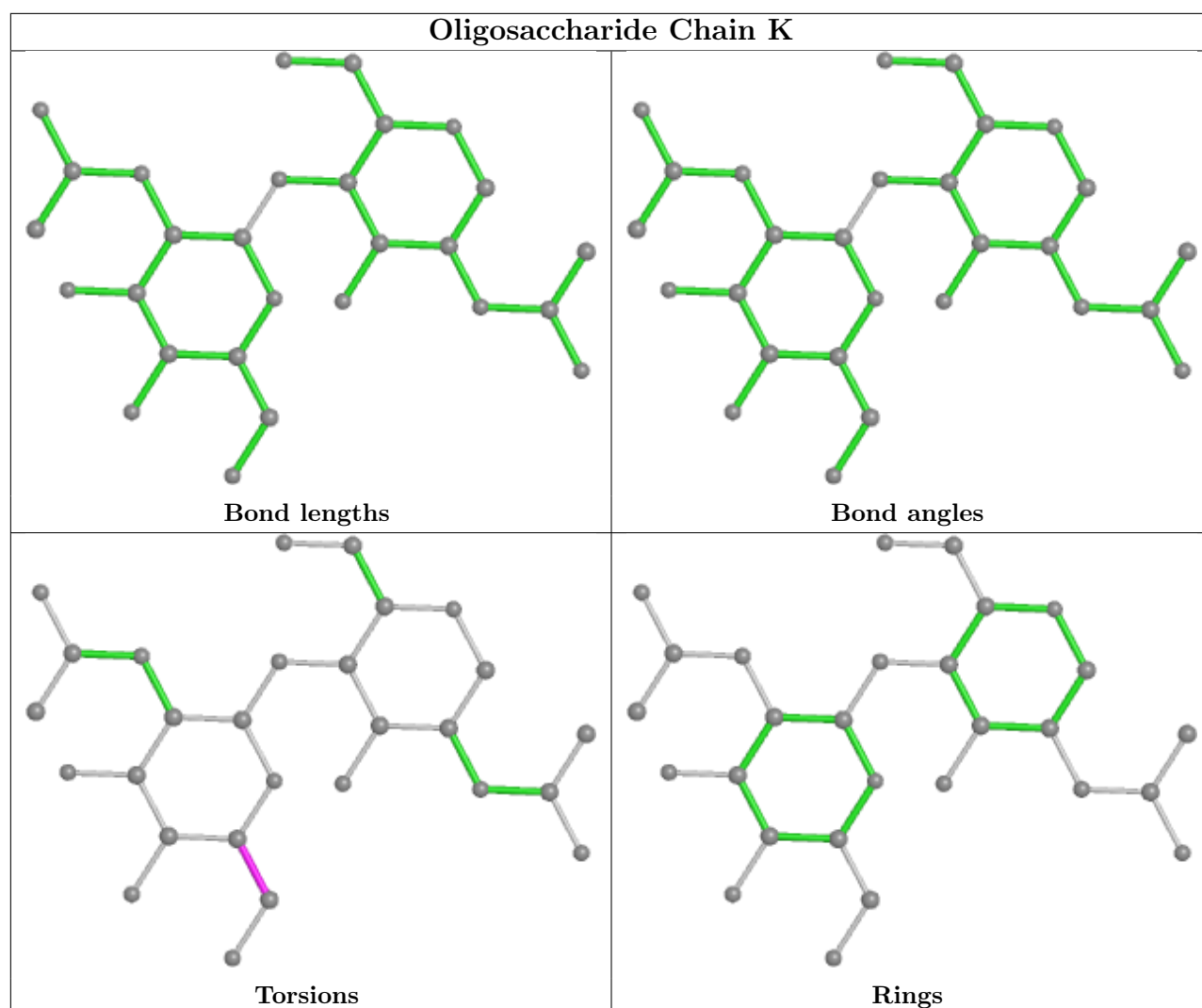


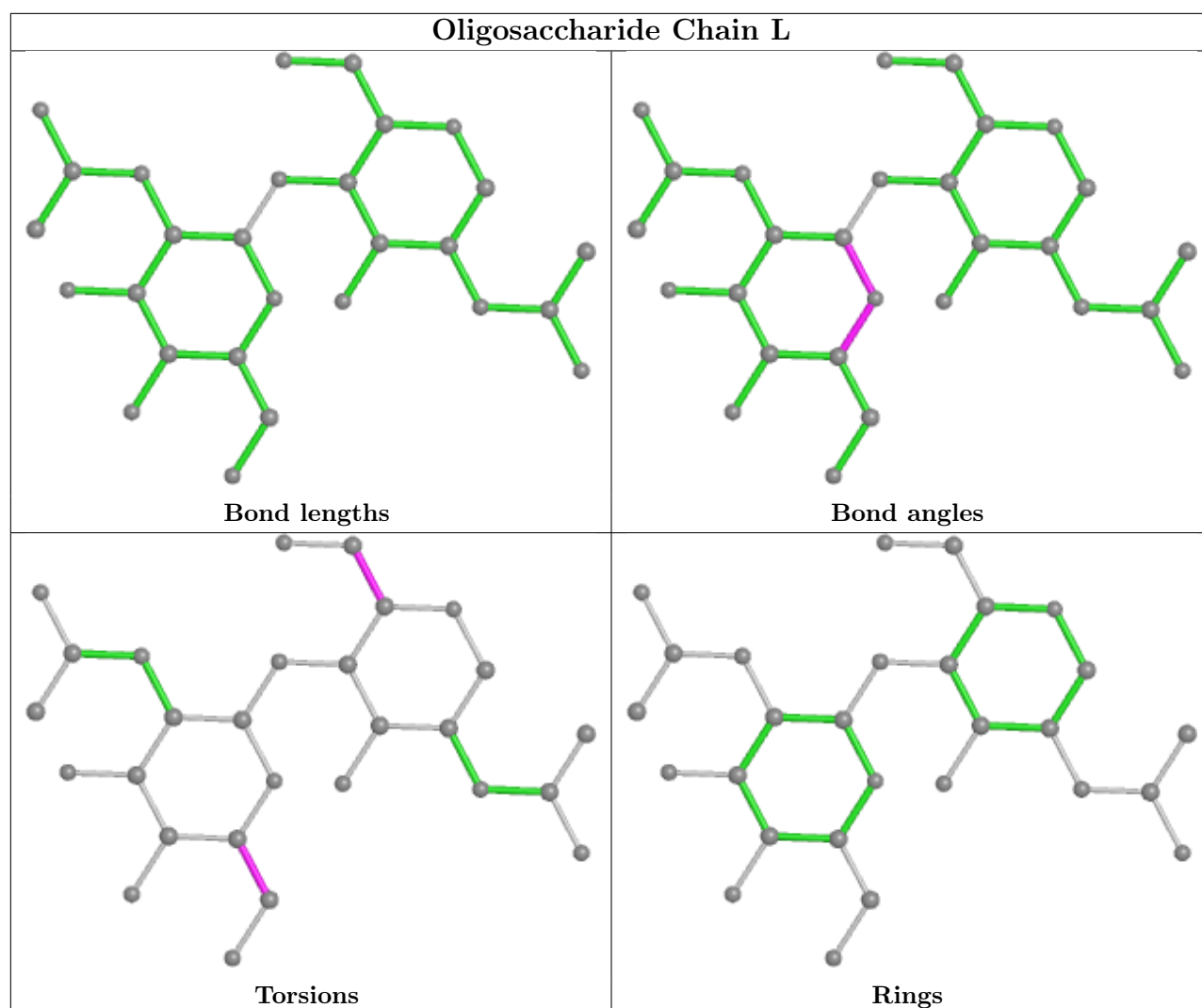


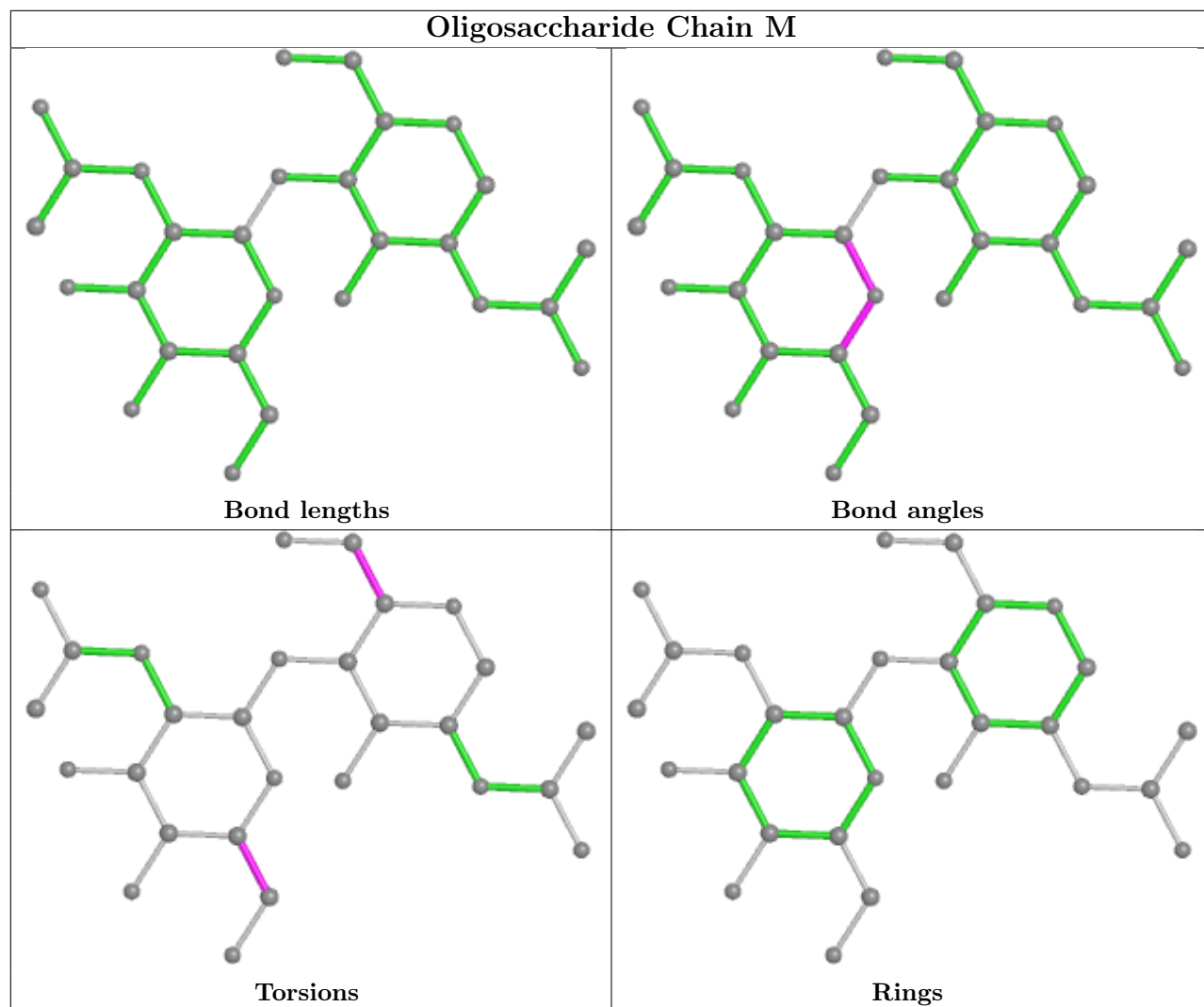


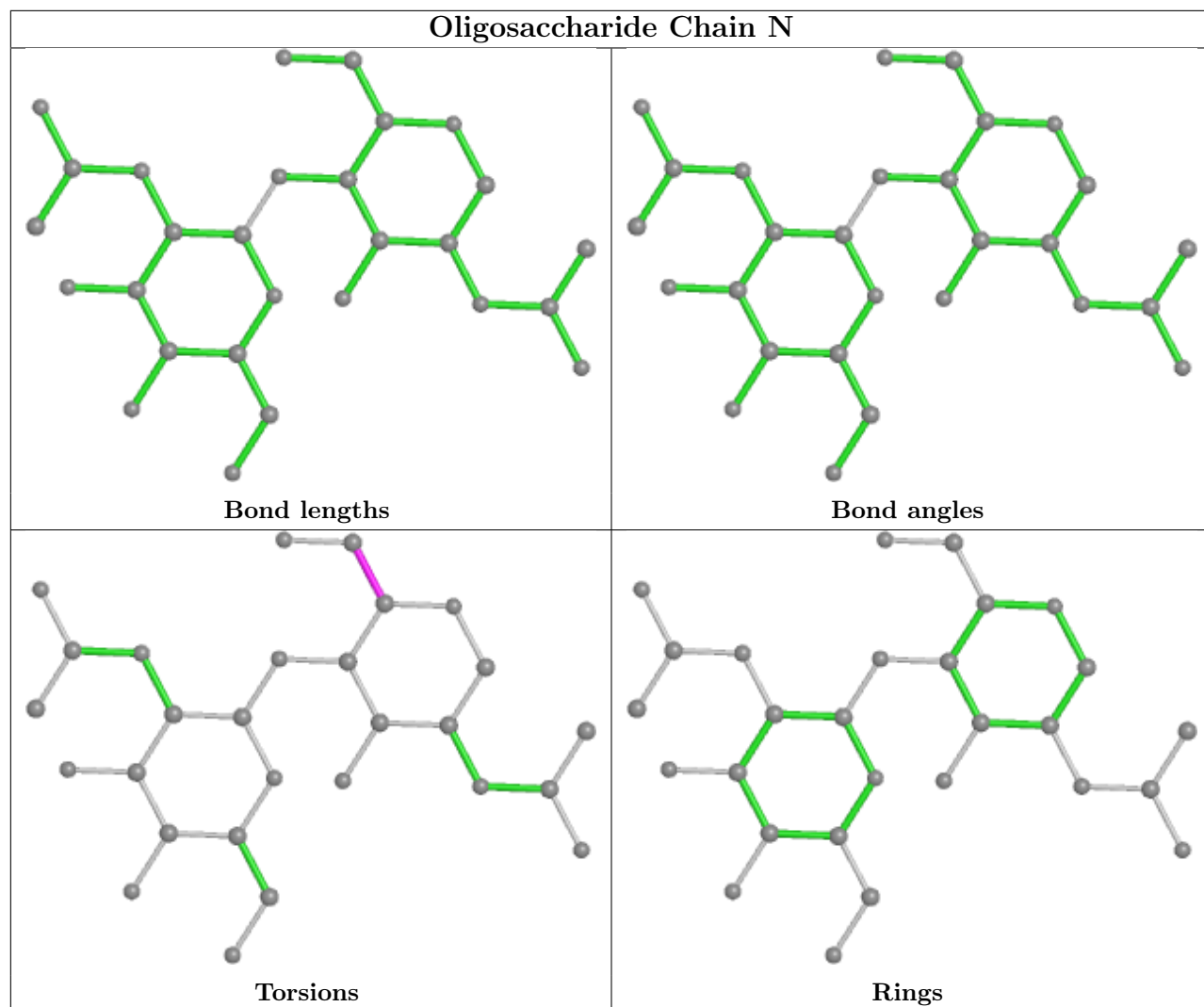


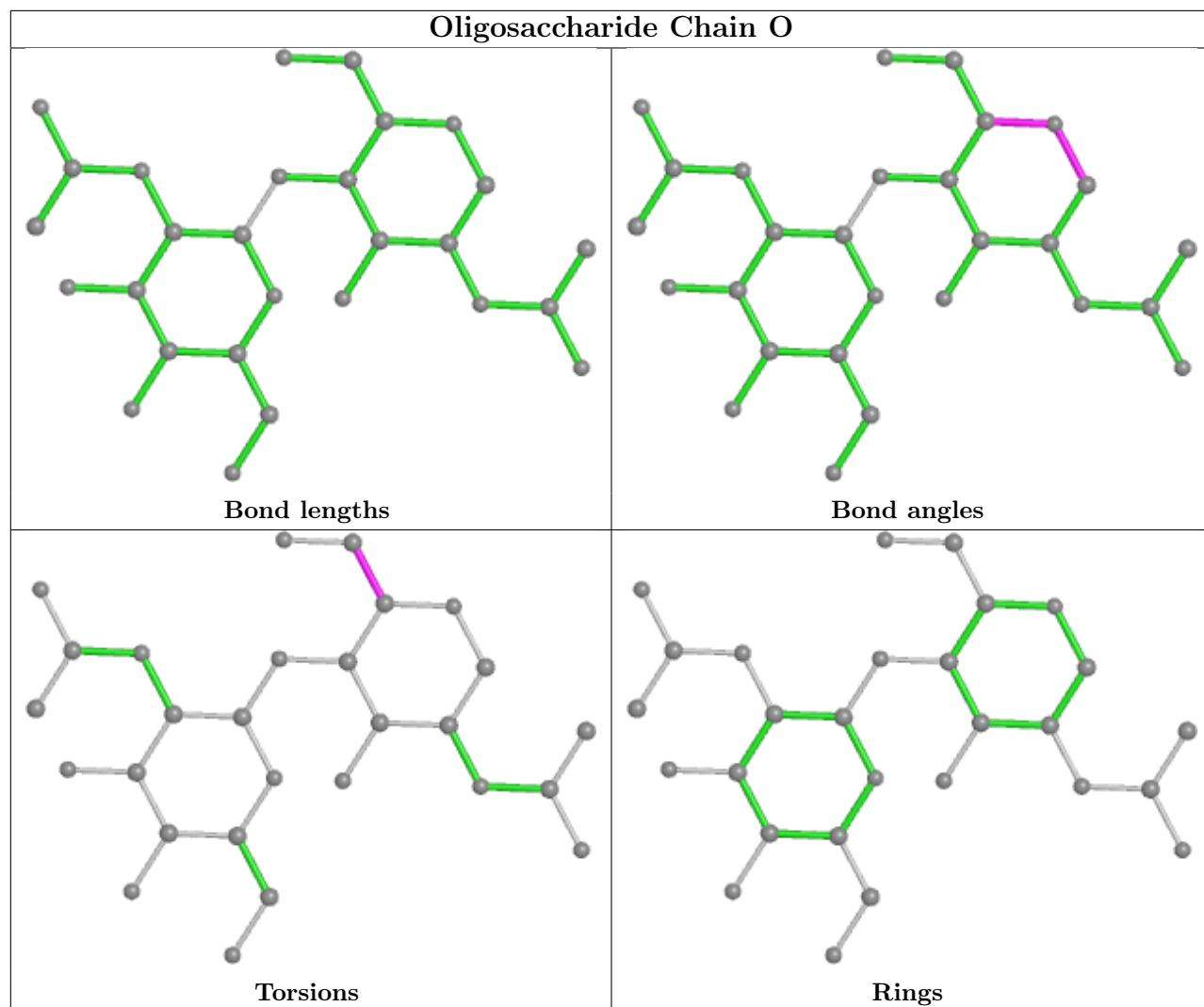


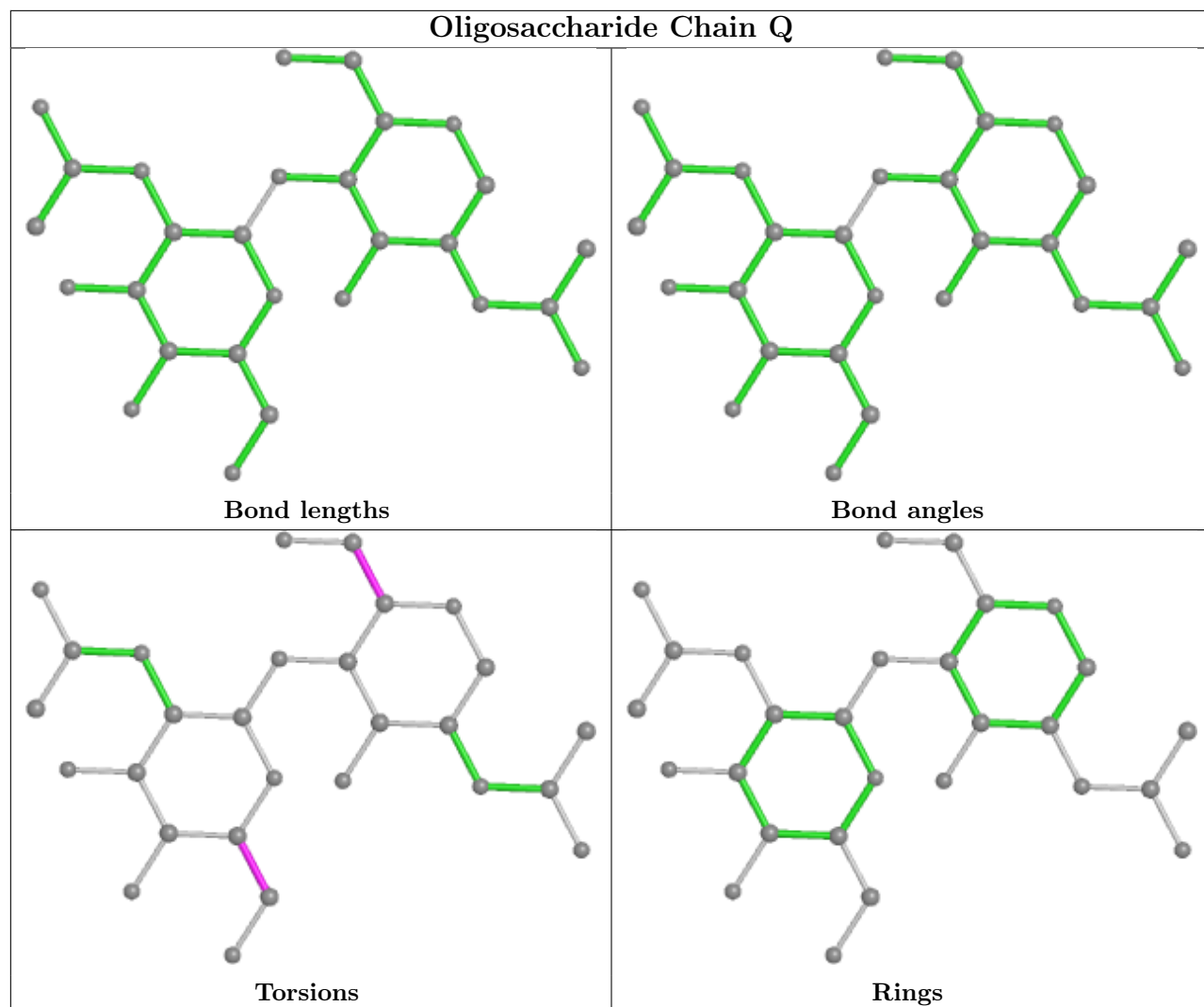


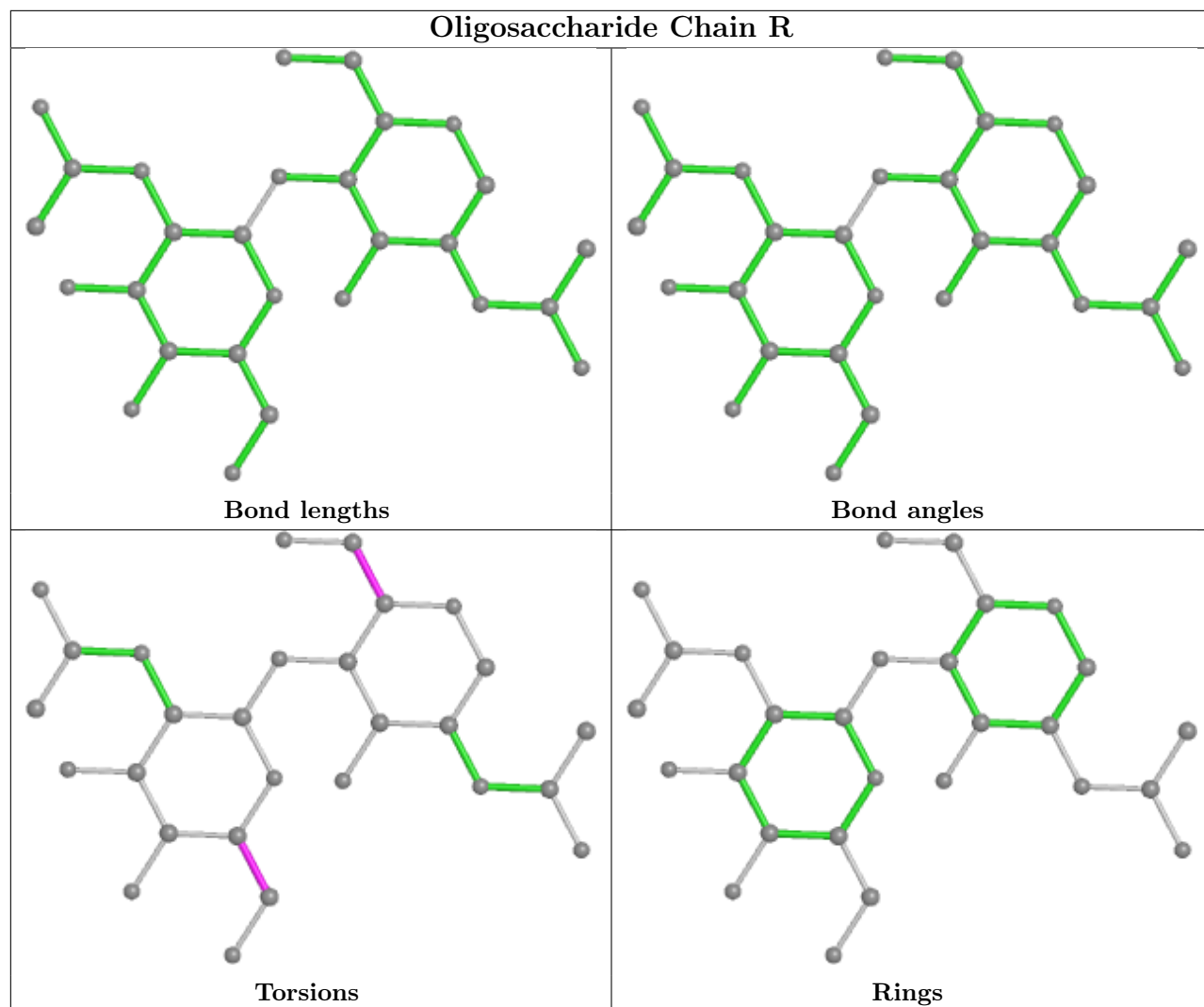


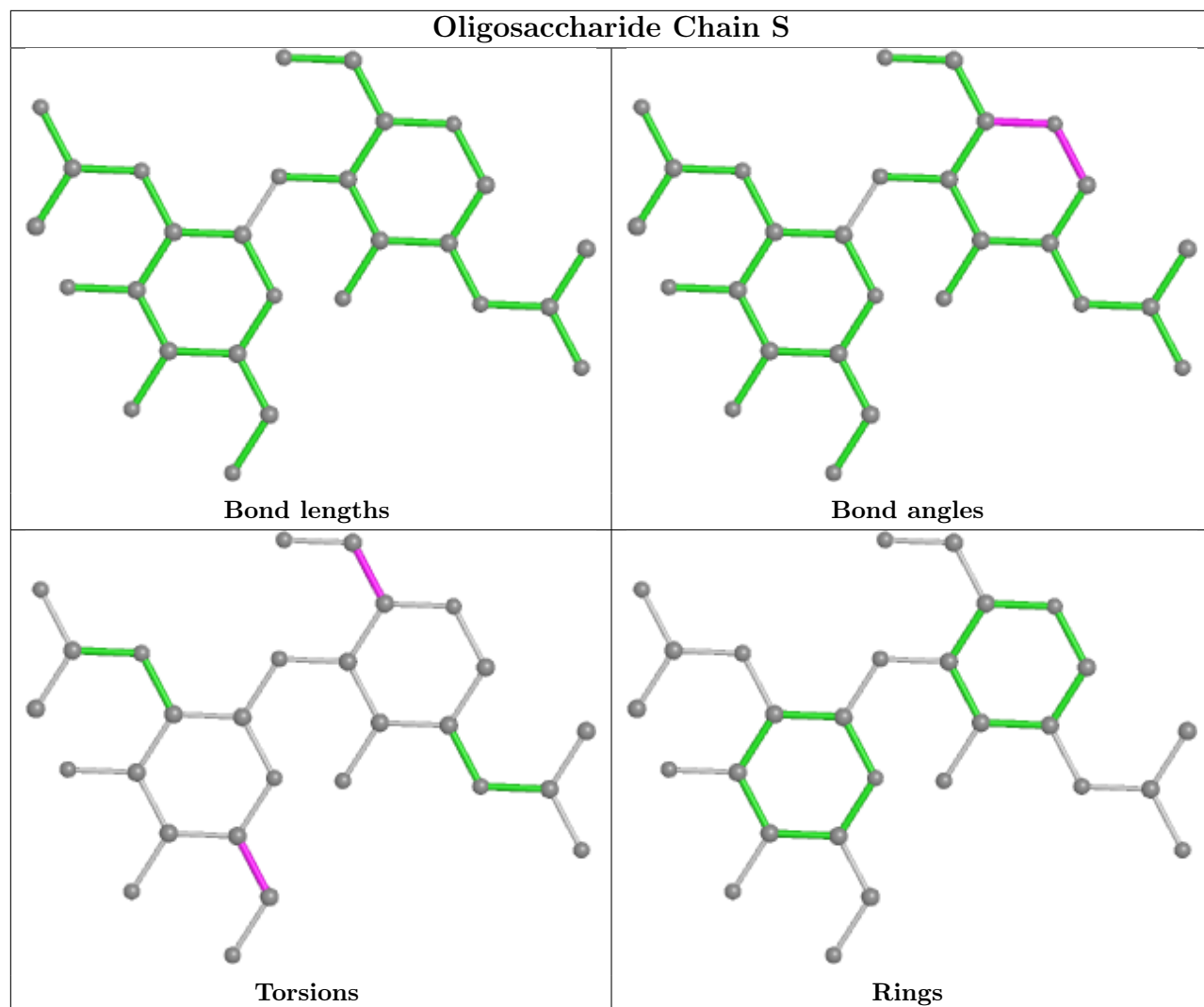


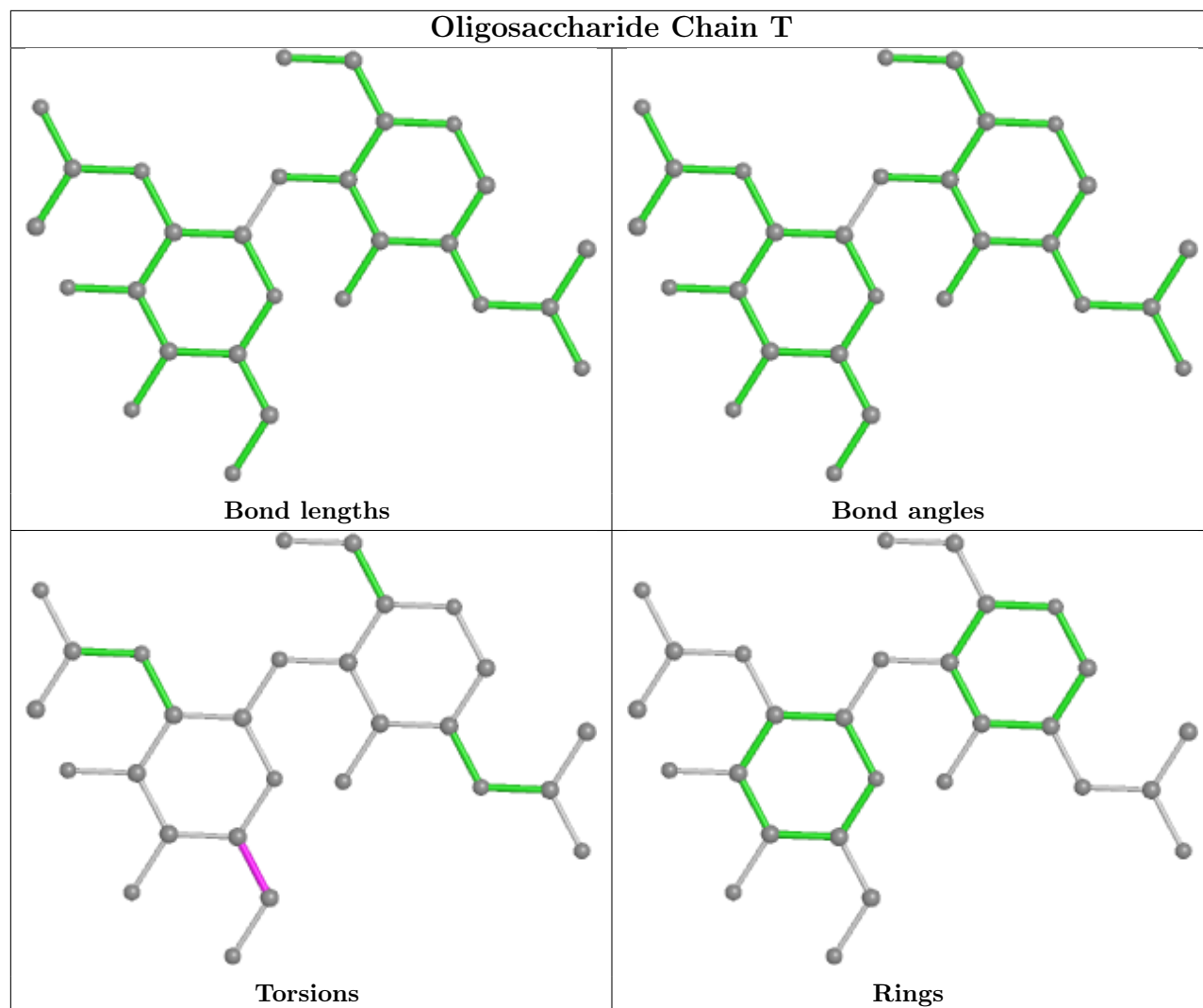


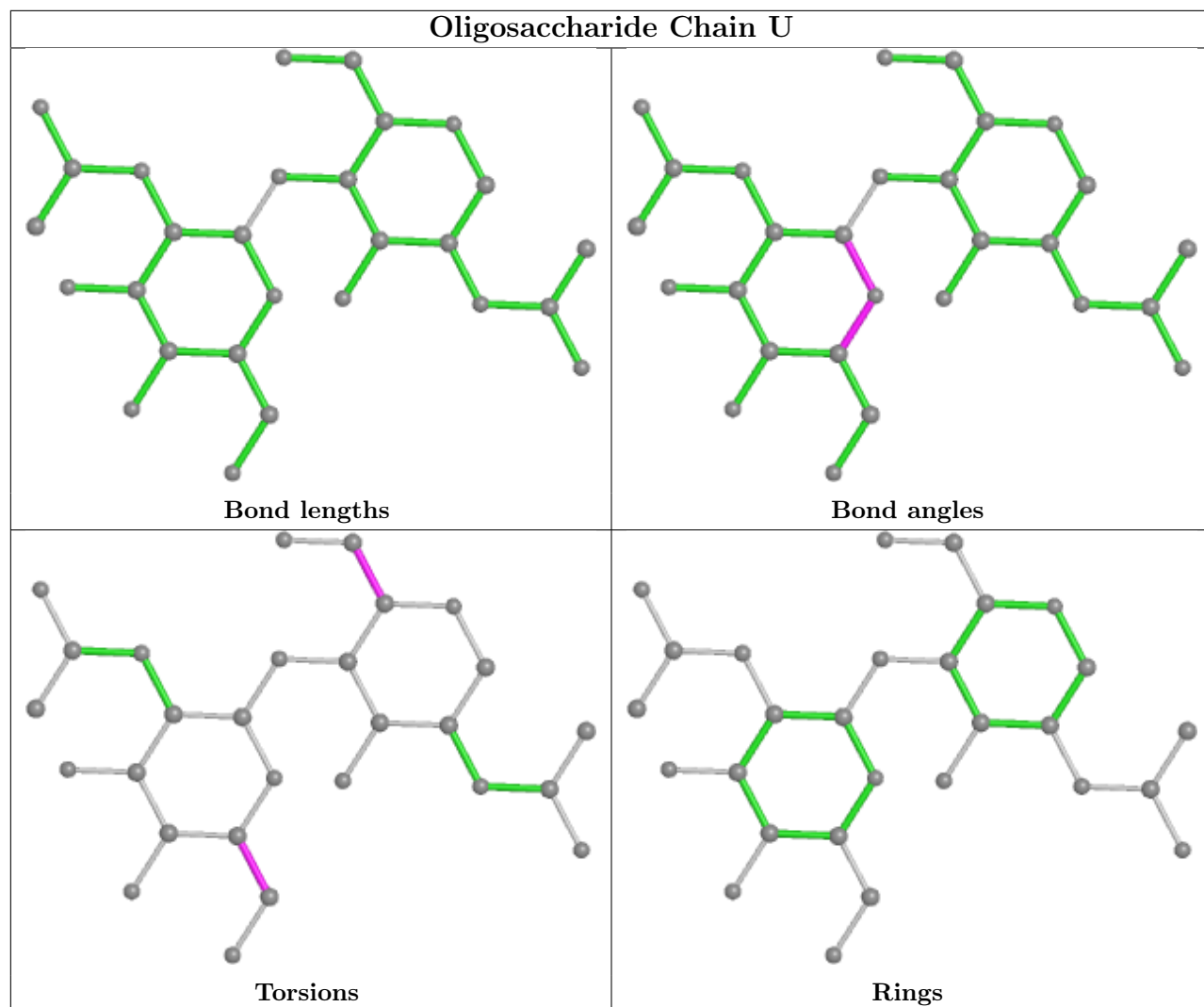


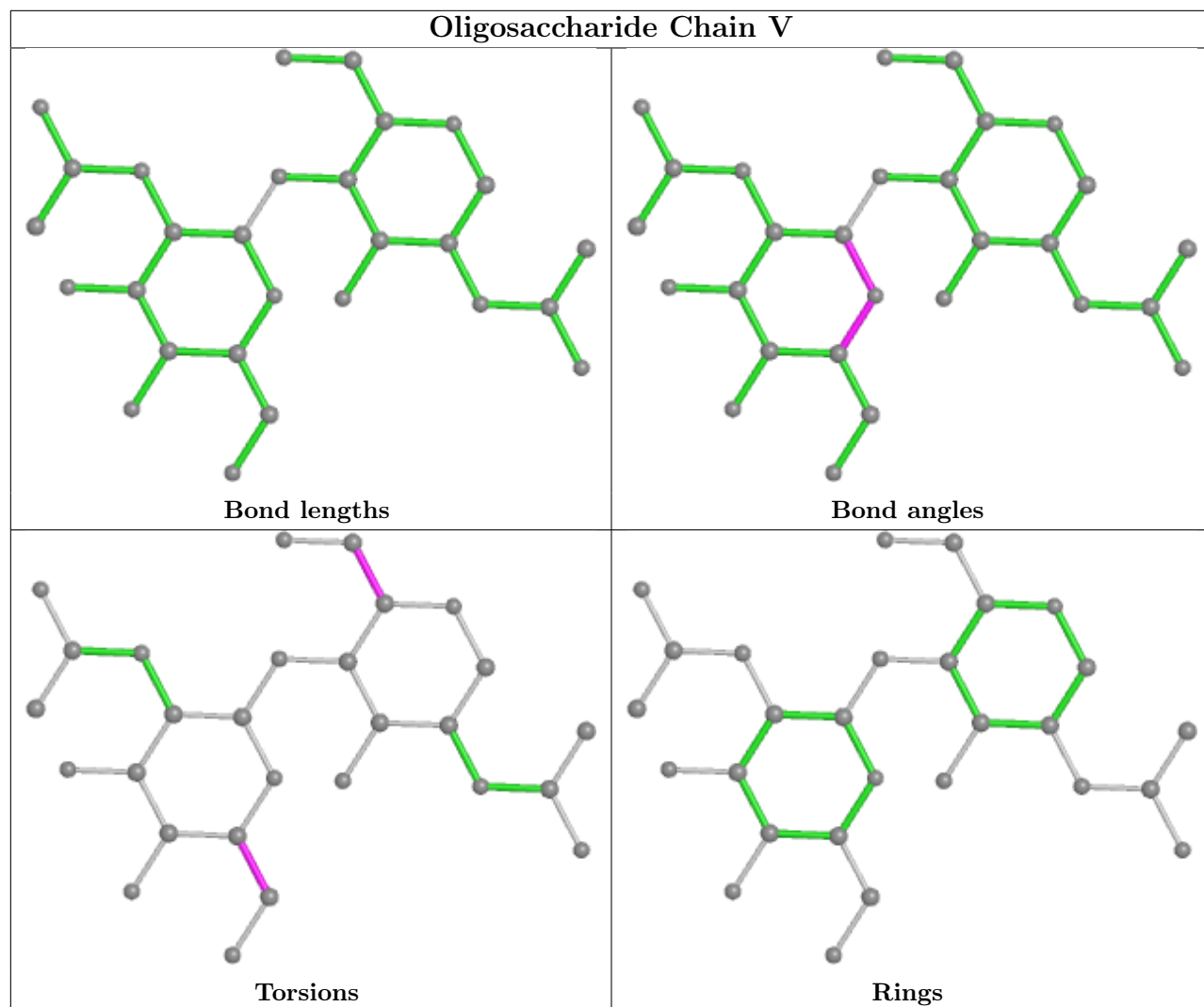


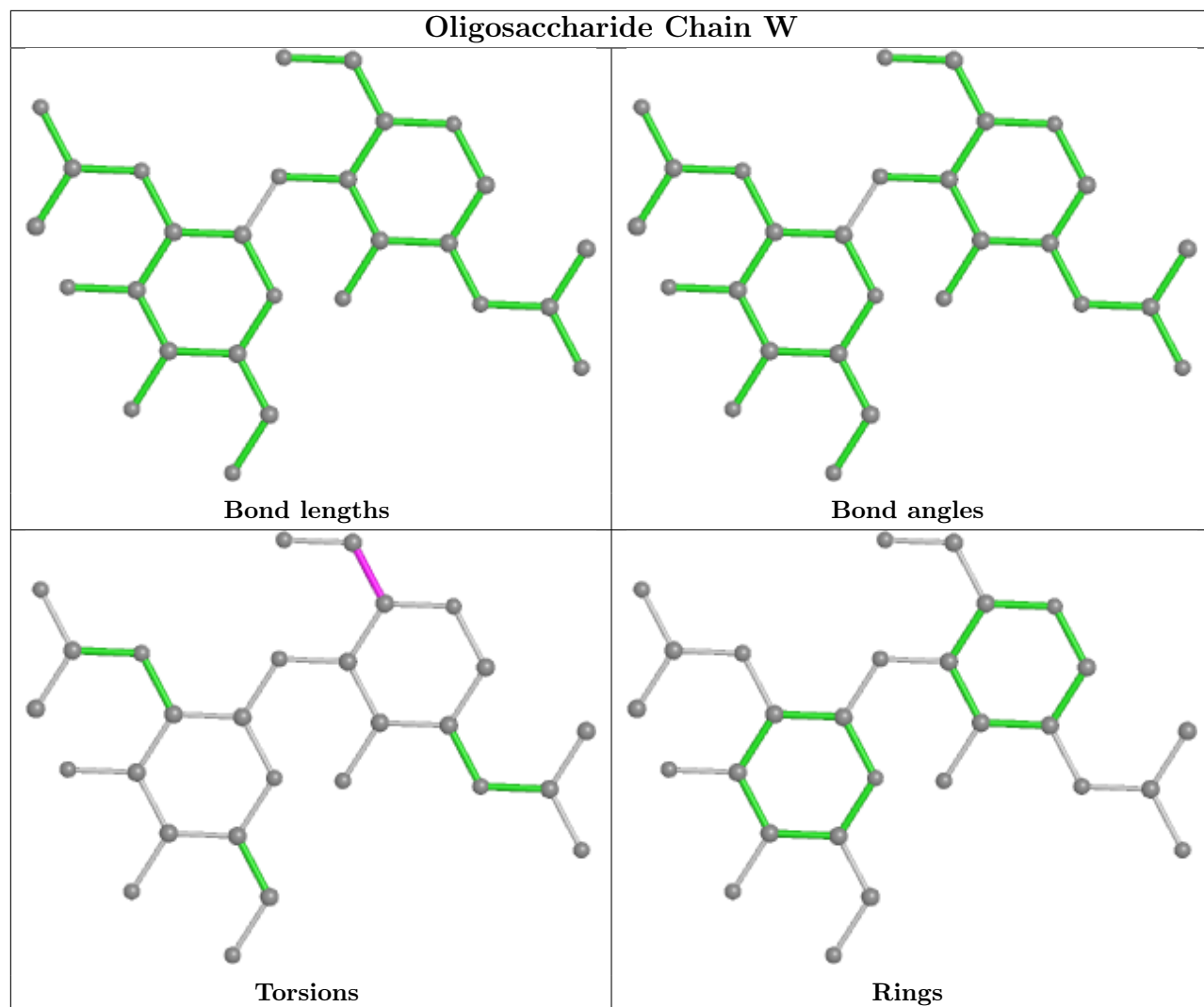


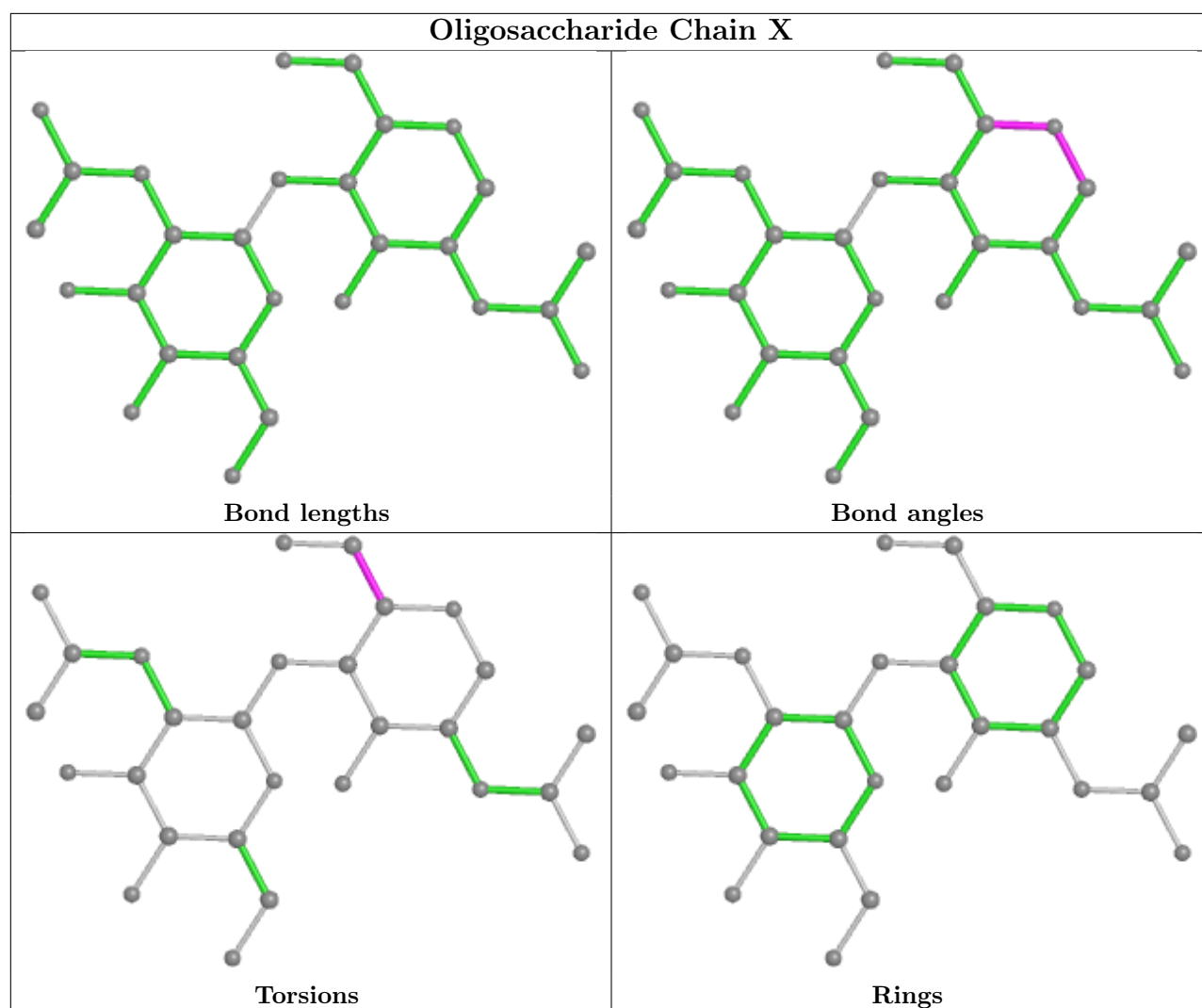


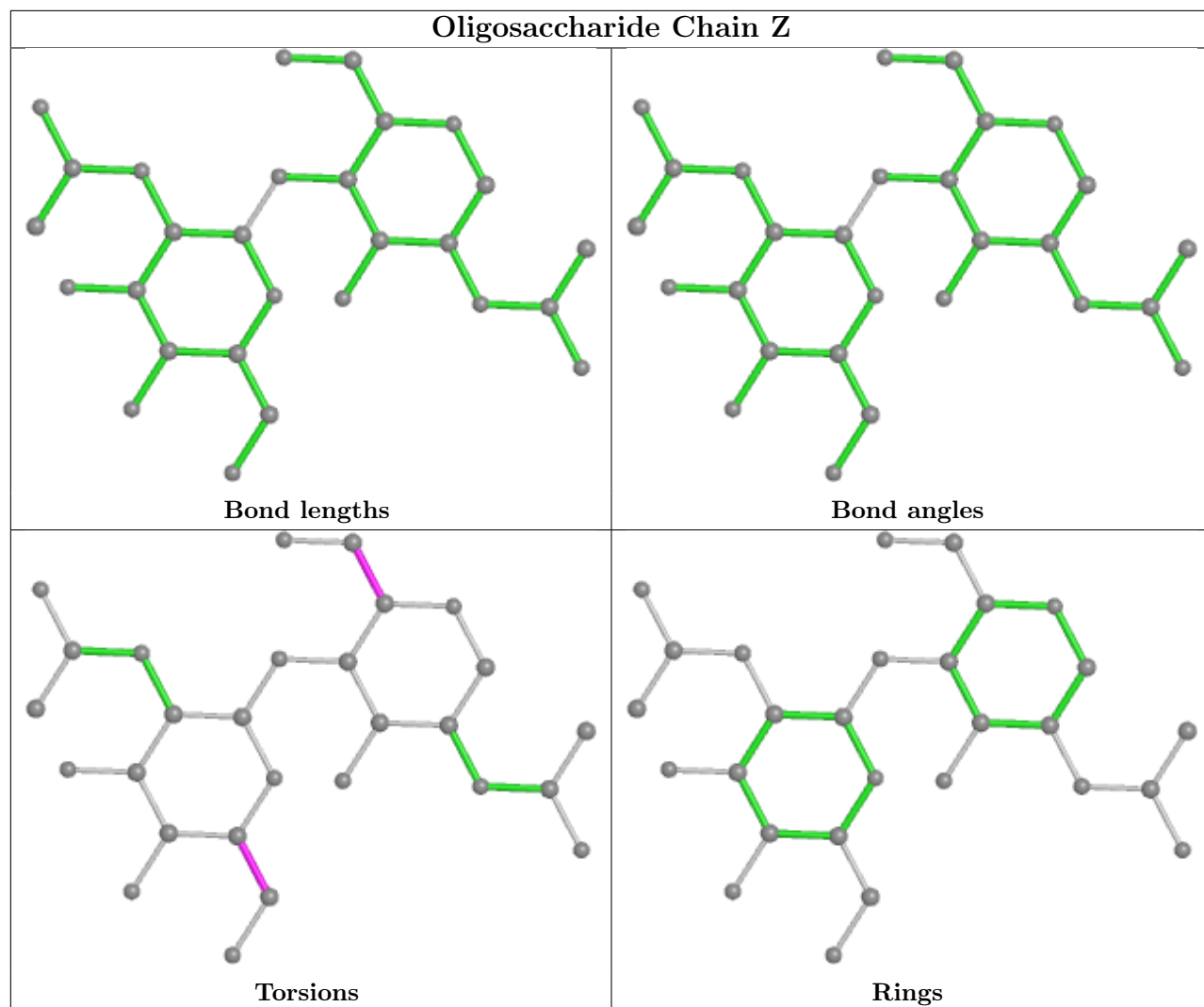


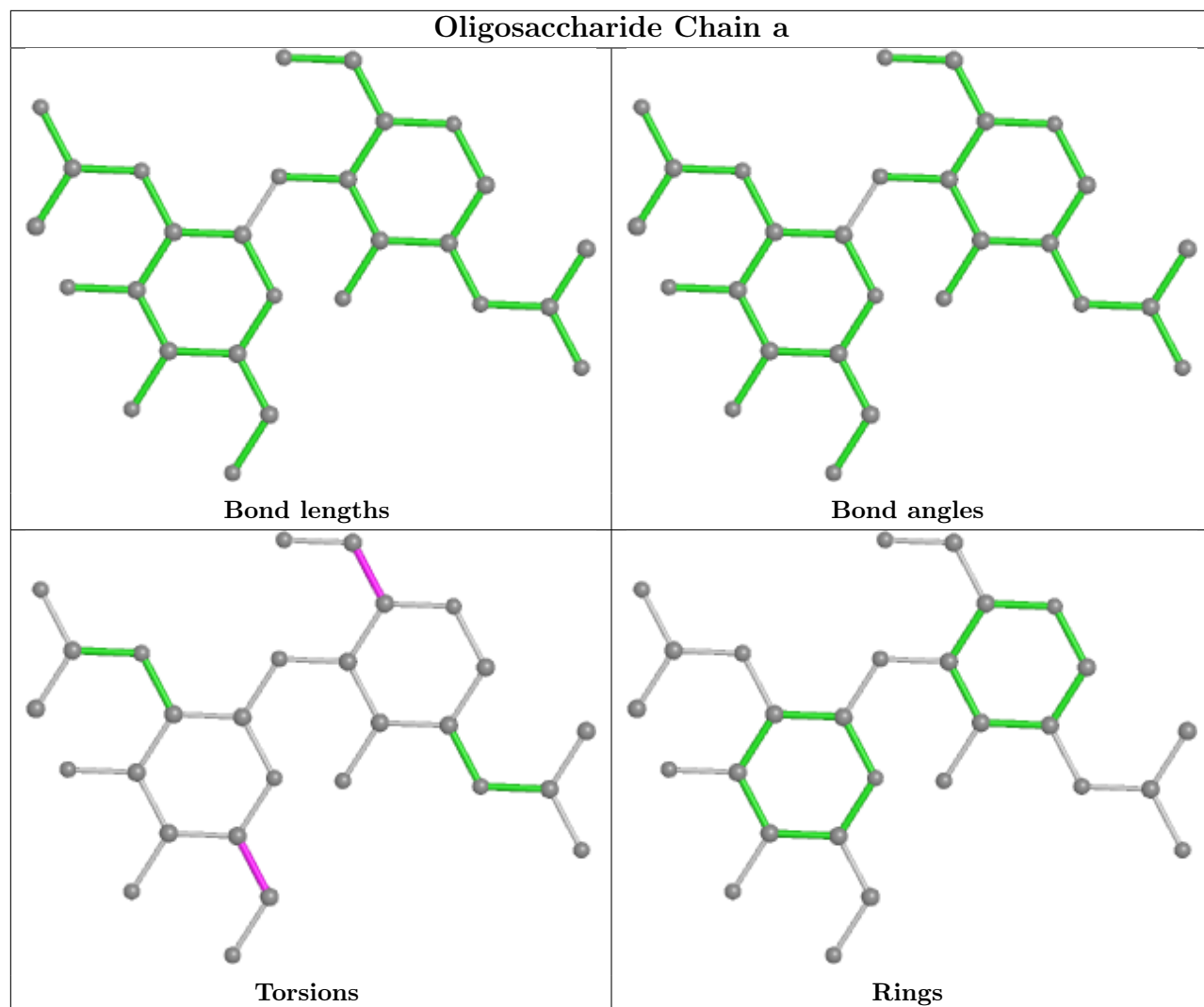


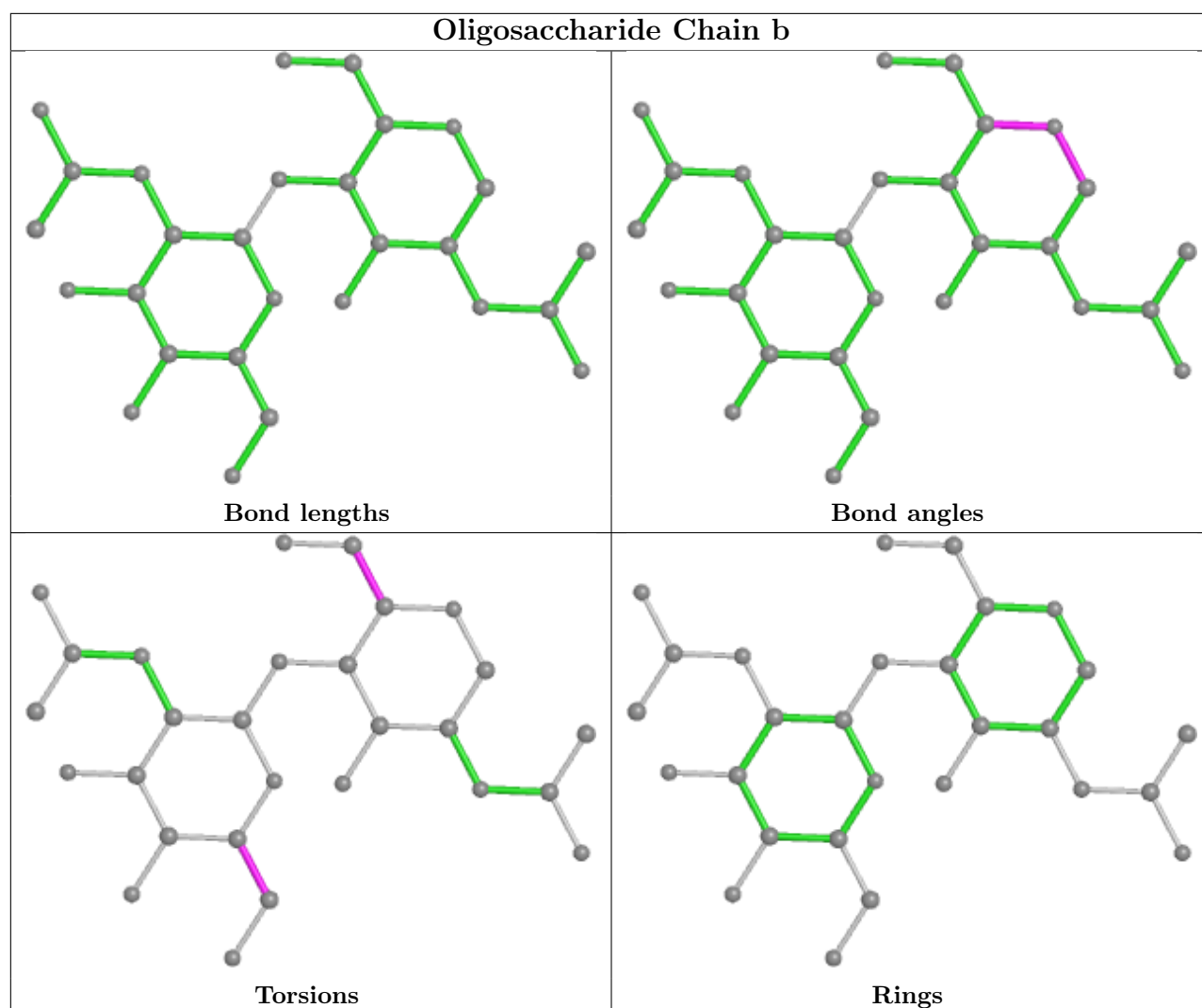


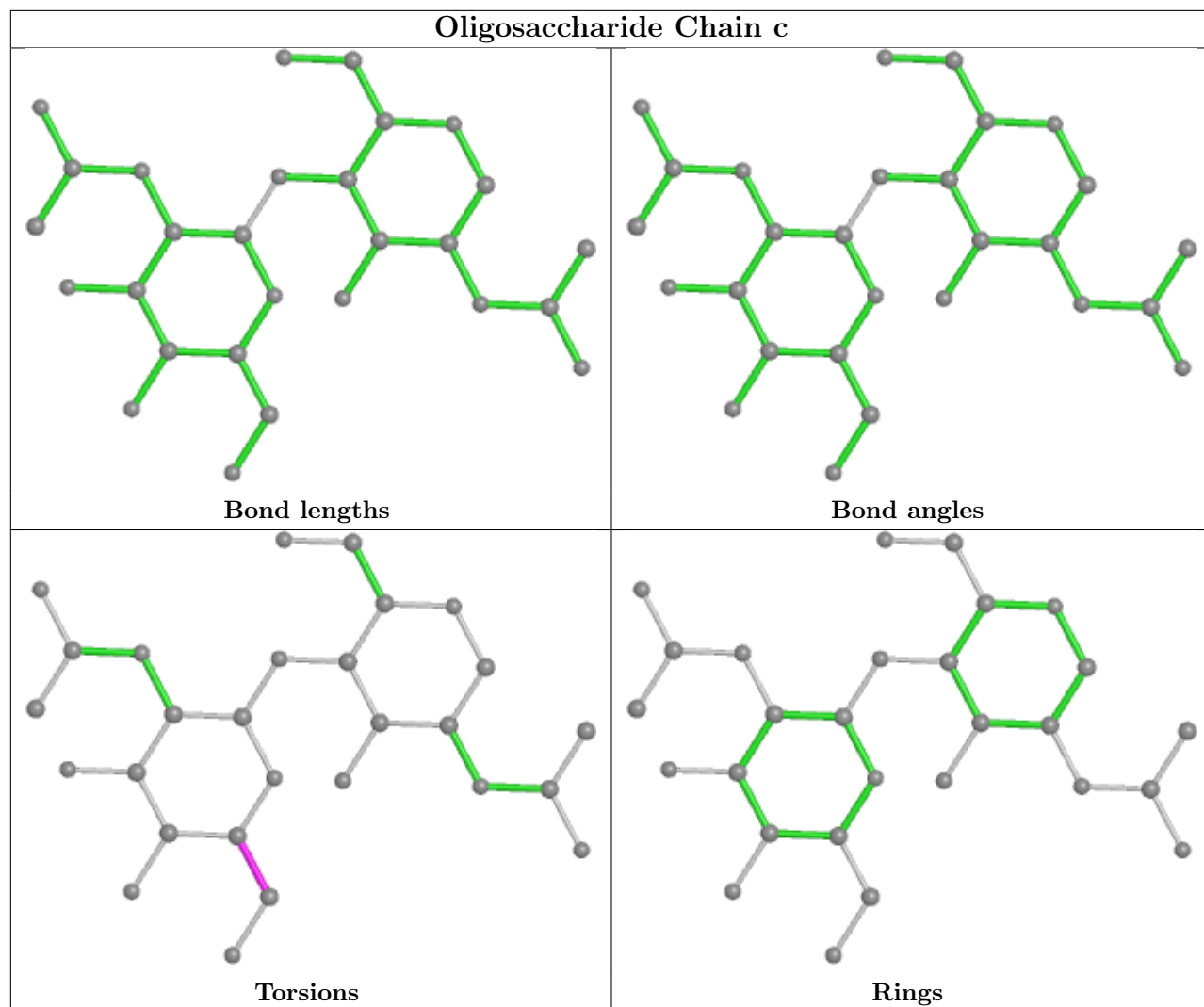


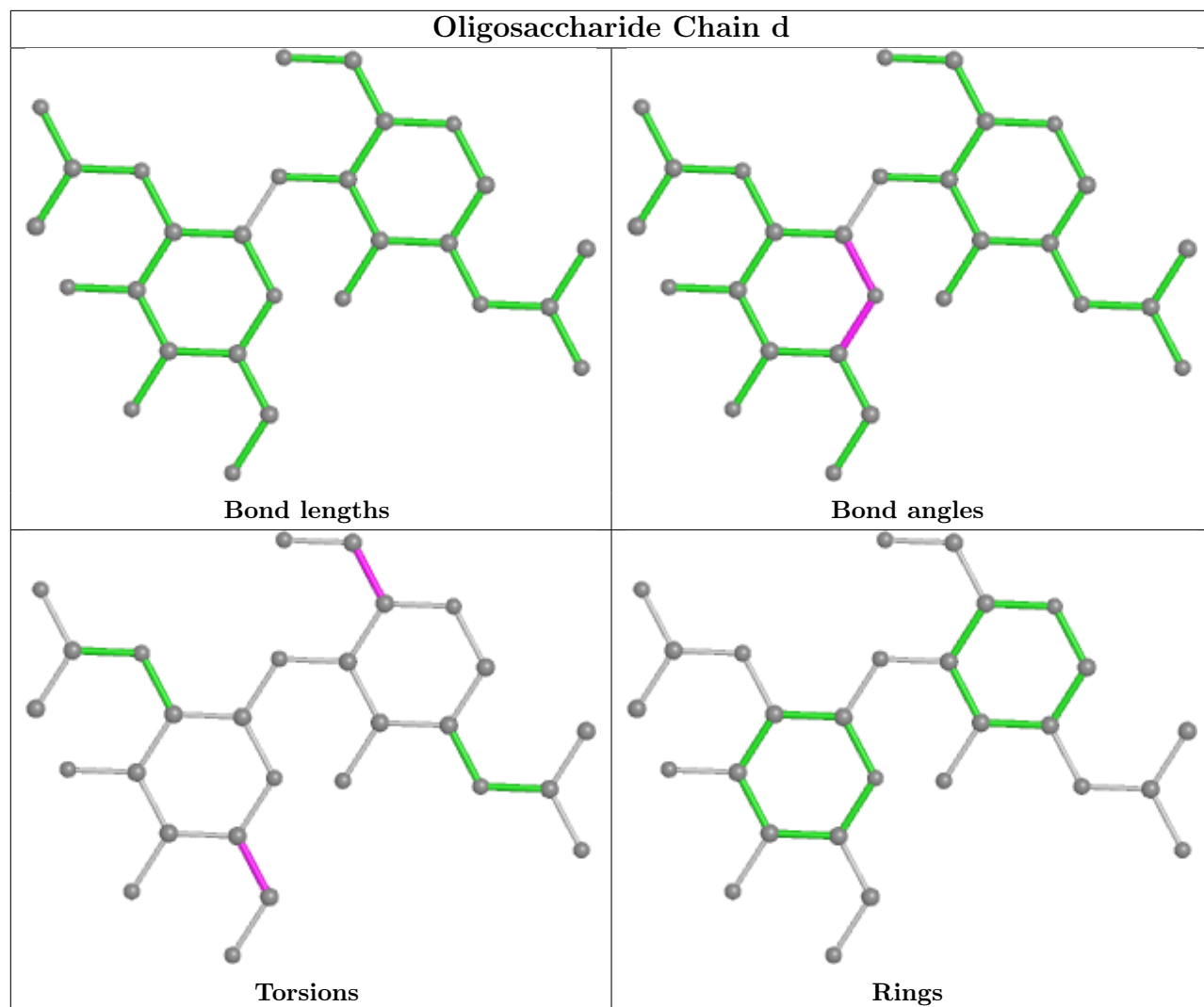


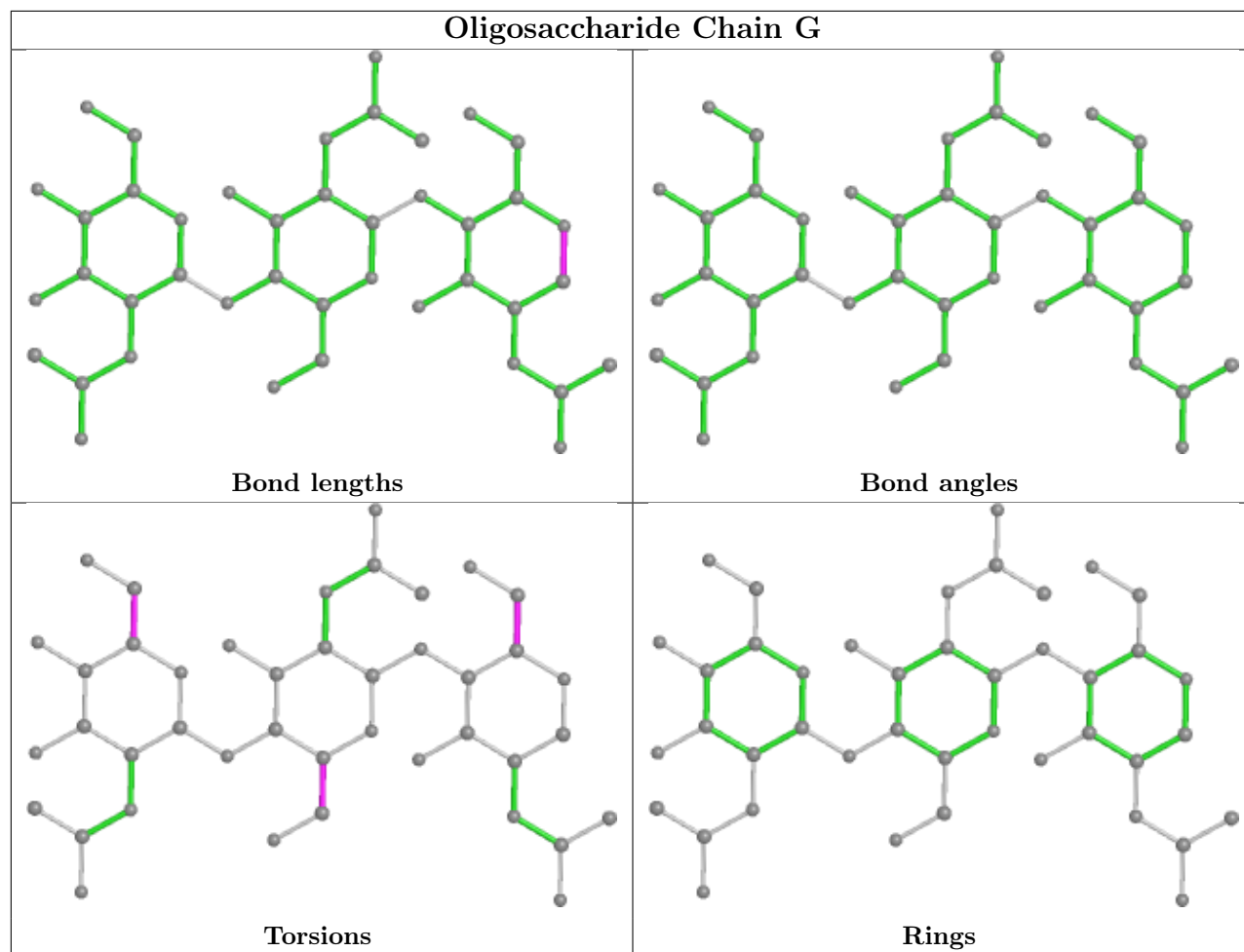


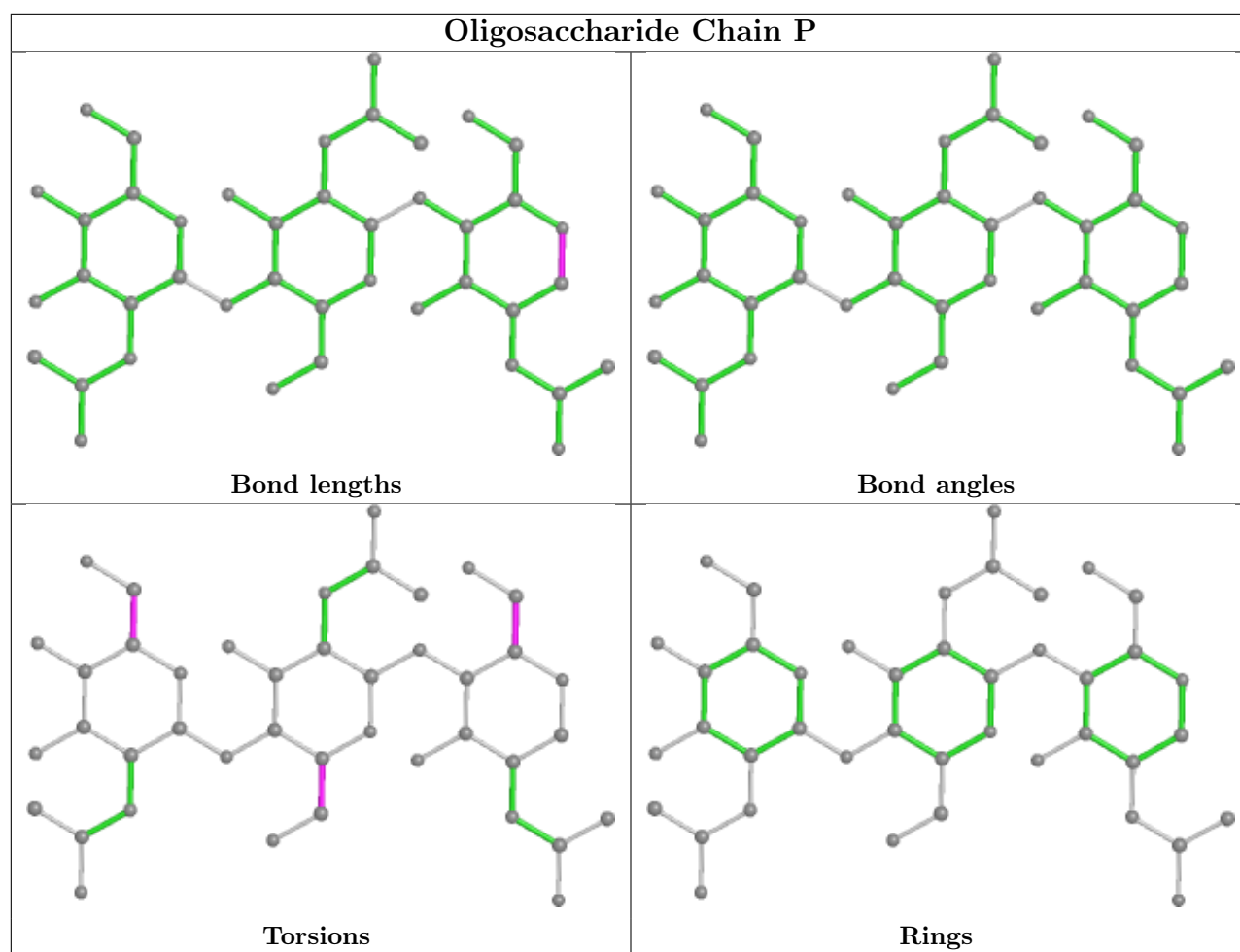


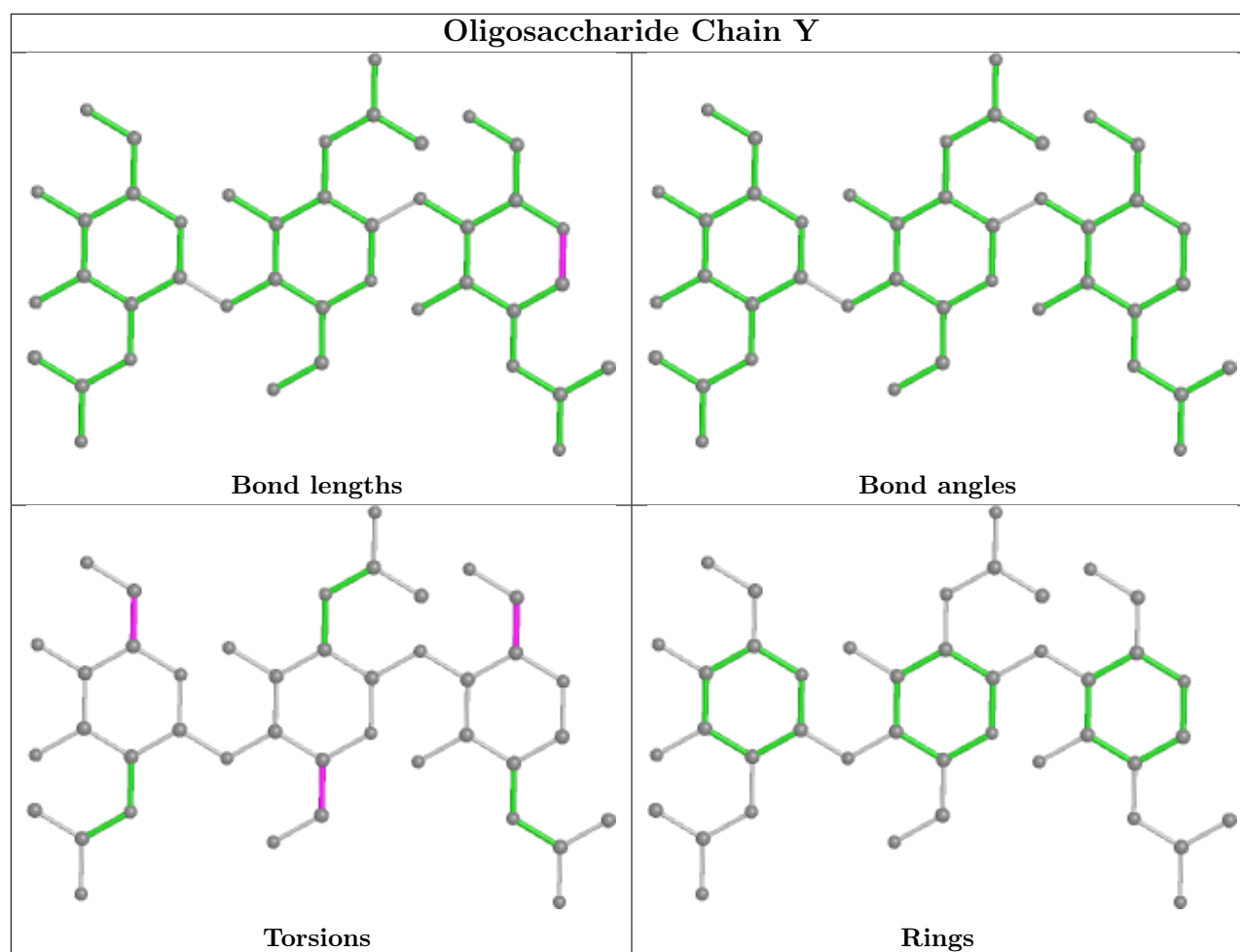












5.6 Ligand geometry [i](#)

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	A	3002	1	14,14,15	0.48	0	17,19,21	0.40	0
5	NAG	A	3005	1	14,14,15	0.50	0	17,19,21	0.45	0
5	NAG	C	3008	1	14,14,15	0.32	0	17,19,21	0.52	0
5	NAG	B	3010	1	14,14,15	0.55	0	17,19,21	0.46	0
5	NAG	B	3006	1	14,14,15	0.38	0	17,19,21	0.55	0
5	NAG	C	3007	1	14,14,15	0.46	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	3007	1	14,14,15	0.46	0	17,19,21	0.54	0
5	NAG	B	3011	1	14,14,15	0.49	0	17,19,21	0.71	1 (5%)
5	NAG	B	3003	1	14,14,15	0.37	0	17,19,21	0.46	0
4	PLM	C	3001	-	17,17,17	0.54	1 (5%)	17,17,17	0.86	0
5	NAG	A	3010	1	14,14,15	0.54	0	17,19,21	0.45	0
5	NAG	B	3009	1	14,14,15	0.44	0	17,19,21	0.41	0
5	NAG	B	3004	1	14,14,15	0.30	0	17,19,21	0.61	1 (5%)
5	NAG	B	3002	1	14,14,15	0.48	0	17,19,21	0.40	0
4	PLM	A	3001	-	17,17,17	0.54	0	17,17,17	0.86	0
5	NAG	B	3008	1	14,14,15	0.34	0	17,19,21	0.52	0
5	NAG	A	3009	1	14,14,15	0.42	0	17,19,21	0.41	0
5	NAG	C	3010	1	14,14,15	0.53	0	17,19,21	0.47	0
5	NAG	A	3008	1	14,14,15	0.32	0	17,19,21	0.52	0
5	NAG	C	3009	1	14,14,15	0.41	0	17,19,21	0.41	0
5	NAG	C	3006	1	14,14,15	0.37	0	17,19,21	0.55	0
5	NAG	A	3004	1	14,14,15	0.30	0	17,19,21	0.62	1 (5%)
4	PLM	B	3001	-	17,17,17	0.53	0	17,17,17	0.86	0
5	NAG	A	3011	1	14,14,15	0.49	0	17,19,21	0.71	1 (5%)
5	NAG	C	3004	1	14,14,15	0.30	0	17,19,21	0.61	1 (5%)
5	NAG	C	3003	1	14,14,15	0.37	0	17,19,21	0.46	0
5	NAG	C	3002	1	14,14,15	0.47	0	17,19,21	0.40	0
5	NAG	C	3005	1	14,14,15	0.51	0	17,19,21	0.45	0
5	NAG	B	3005	1	14,14,15	0.51	0	17,19,21	0.44	0
5	NAG	A	3006	1	14,14,15	0.37	0	17,19,21	0.55	0
5	NAG	A	3007	1	14,14,15	0.48	0	17,19,21	0.54	0
5	NAG	C	3011	1	14,14,15	0.48	0	17,19,21	0.71	1 (5%)
5	NAG	A	3003	1	14,14,15	0.37	0	17,19,21	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	3002	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3005	1	-	2/6/23/26	0/1/1/1
5	NAG	C	3008	1	-	2/6/23/26	0/1/1/1
5	NAG	B	3010	1	-	2/6/23/26	0/1/1/1
5	NAG	B	3006	1	-	0/6/23/26	0/1/1/1
5	NAG	C	3007	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	3007	1	-	1/6/23/26	0/1/1/1
5	NAG	B	3011	1	-	1/6/23/26	0/1/1/1
5	NAG	B	3003	1	-	0/6/23/26	0/1/1/1
4	PLM	C	3001	-	-	7/15/15/15	-
5	NAG	A	3010	1	-	2/6/23/26	0/1/1/1
5	NAG	B	3009	1	-	2/6/23/26	0/1/1/1
5	NAG	B	3004	1	-	2/6/23/26	0/1/1/1
5	NAG	B	3002	1	-	2/6/23/26	0/1/1/1
4	PLM	A	3001	-	-	7/15/15/15	-
5	NAG	B	3008	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3009	1	-	2/6/23/26	0/1/1/1
5	NAG	C	3010	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3008	1	-	2/6/23/26	0/1/1/1
5	NAG	C	3009	1	-	2/6/23/26	0/1/1/1
5	NAG	C	3006	1	-	0/6/23/26	0/1/1/1
5	NAG	A	3004	1	-	2/6/23/26	0/1/1/1
4	PLM	B	3001	-	-	7/15/15/15	-
5	NAG	A	3011	1	-	1/6/23/26	0/1/1/1
5	NAG	C	3004	1	-	2/6/23/26	0/1/1/1
5	NAG	C	3003	1	-	0/6/23/26	0/1/1/1
5	NAG	C	3002	1	-	2/6/23/26	0/1/1/1
5	NAG	C	3005	1	-	2/6/23/26	0/1/1/1
5	NAG	B	3005	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3006	1	-	0/6/23/26	0/1/1/1
5	NAG	A	3007	1	-	1/6/23/26	0/1/1/1
5	NAG	C	3011	1	-	1/6/23/26	0/1/1/1
5	NAG	A	3003	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3001	PLM	O1-C1	-2.01	1.24	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3011	NAG	C1-O5-C5	2.56	115.66	112.19
5	B	3011	NAG	C1-O5-C5	2.56	115.66	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3011	NAG	C1-O5-C5	2.55	115.65	112.19
5	A	3004	NAG	C1-O5-C5	2.18	115.15	112.19
5	B	3004	NAG	C1-O5-C5	2.17	115.13	112.19
5	C	3004	NAG	C1-O5-C5	2.14	115.09	112.19

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3004	NAG	O5-C5-C6-O6
5	C	3004	NAG	O5-C5-C6-O6
5	B	3004	NAG	O5-C5-C6-O6
5	A	3004	NAG	C4-C5-C6-O6
5	C	3004	NAG	C4-C5-C6-O6
5	B	3004	NAG	C4-C5-C6-O6
5	A	3010	NAG	O5-C5-C6-O6
5	C	3010	NAG	O5-C5-C6-O6
5	B	3010	NAG	O5-C5-C6-O6
5	A	3010	NAG	C4-C5-C6-O6
5	C	3010	NAG	C4-C5-C6-O6
5	B	3010	NAG	C4-C5-C6-O6
5	A	3002	NAG	O5-C5-C6-O6
5	C	3002	NAG	O5-C5-C6-O6
5	B	3002	NAG	O5-C5-C6-O6
5	C	3009	NAG	C4-C5-C6-O6
5	A	3009	NAG	C4-C5-C6-O6
5	B	3009	NAG	C4-C5-C6-O6
4	A	3001	PLM	C7-C8-C9-CA
4	C	3001	PLM	C7-C8-C9-CA
4	B	3001	PLM	C7-C8-C9-CA
4	A	3001	PLM	C4-C5-C6-C7
4	C	3001	PLM	C4-C5-C6-C7
4	B	3001	PLM	C4-C5-C6-C7
4	A	3001	PLM	C6-C7-C8-C9
4	C	3001	PLM	C6-C7-C8-C9
4	B	3001	PLM	C6-C7-C8-C9
5	A	3009	NAG	O5-C5-C6-O6
5	C	3009	NAG	O5-C5-C6-O6
5	B	3009	NAG	O5-C5-C6-O6
5	A	3007	NAG	O5-C5-C6-O6
5	C	3007	NAG	O5-C5-C6-O6
5	B	3007	NAG	O5-C5-C6-O6

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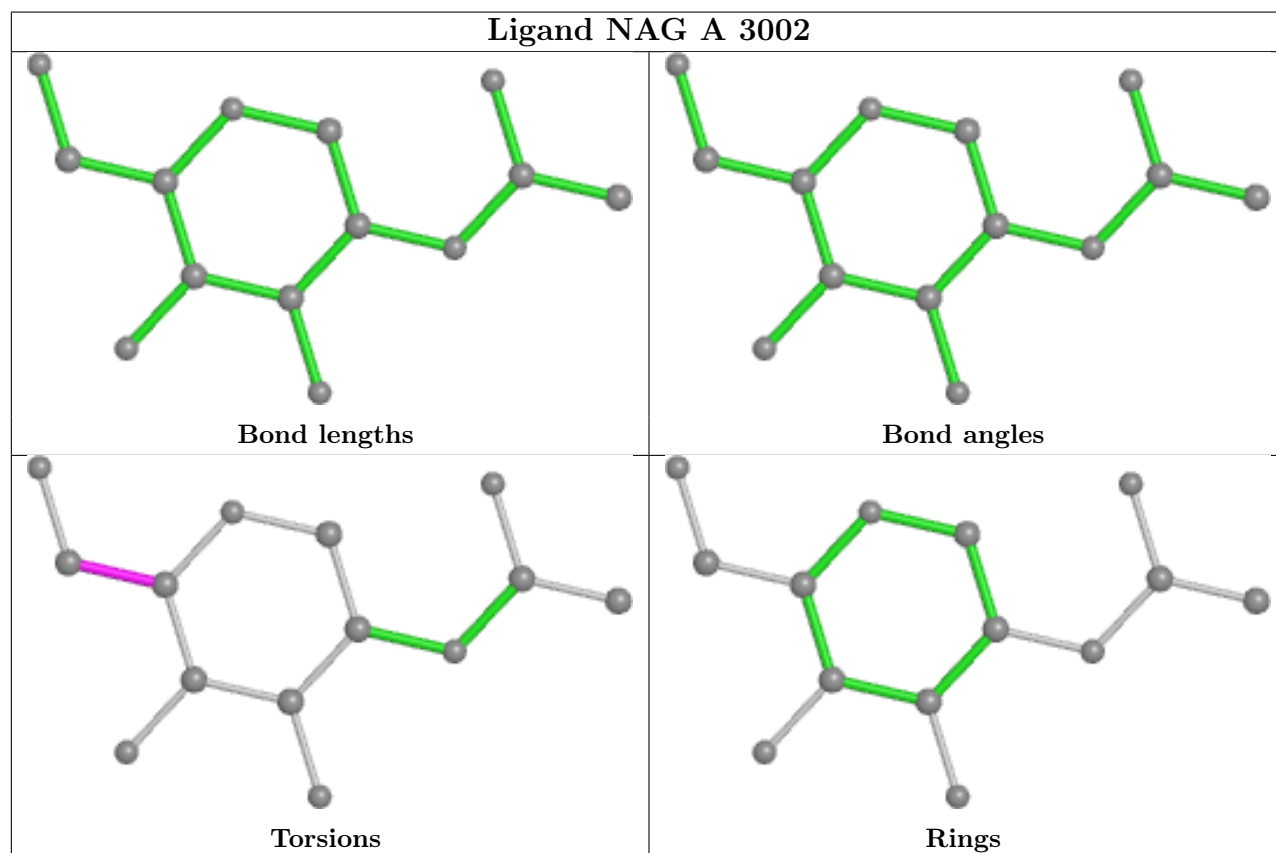
Mol	Chain	Res	Type	Atoms
5	A	3011	NAG	O5-C5-C6-O6
5	C	3011	NAG	O5-C5-C6-O6
5	B	3011	NAG	O5-C5-C6-O6
4	C	3001	PLM	C9-CA-CB-CC
4	A	3001	PLM	C9-CA-CB-CC
4	B	3001	PLM	C9-CA-CB-CC
5	A	3005	NAG	C4-C5-C6-O6
5	B	3005	NAG	C4-C5-C6-O6
5	C	3005	NAG	C4-C5-C6-O6
4	A	3001	PLM	C2-C3-C4-C5
4	C	3001	PLM	C2-C3-C4-C5
4	B	3001	PLM	C2-C3-C4-C5
5	A	3002	NAG	C4-C5-C6-O6
5	C	3002	NAG	C4-C5-C6-O6
5	B	3002	NAG	C4-C5-C6-O6
5	A	3008	NAG	C4-C5-C6-O6
5	C	3008	NAG	C4-C5-C6-O6
5	B	3008	NAG	C4-C5-C6-O6
4	A	3001	PLM	O1-C1-C2-C3
4	C	3001	PLM	O1-C1-C2-C3
4	B	3001	PLM	O1-C1-C2-C3
5	A	3005	NAG	O5-C5-C6-O6
5	C	3005	NAG	O5-C5-C6-O6
5	B	3005	NAG	O5-C5-C6-O6
4	C	3001	PLM	O2-C1-C2-C3
4	A	3001	PLM	O2-C1-C2-C3
4	B	3001	PLM	O2-C1-C2-C3
5	B	3008	NAG	O5-C5-C6-O6
5	A	3008	NAG	O5-C5-C6-O6
5	C	3008	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3001	PLM	2	0
5	B	3009	NAG	1	0
4	A	3001	PLM	2	0
5	A	3009	NAG	1	0
5	C	3009	NAG	1	0
4	B	3001	PLM	3	0

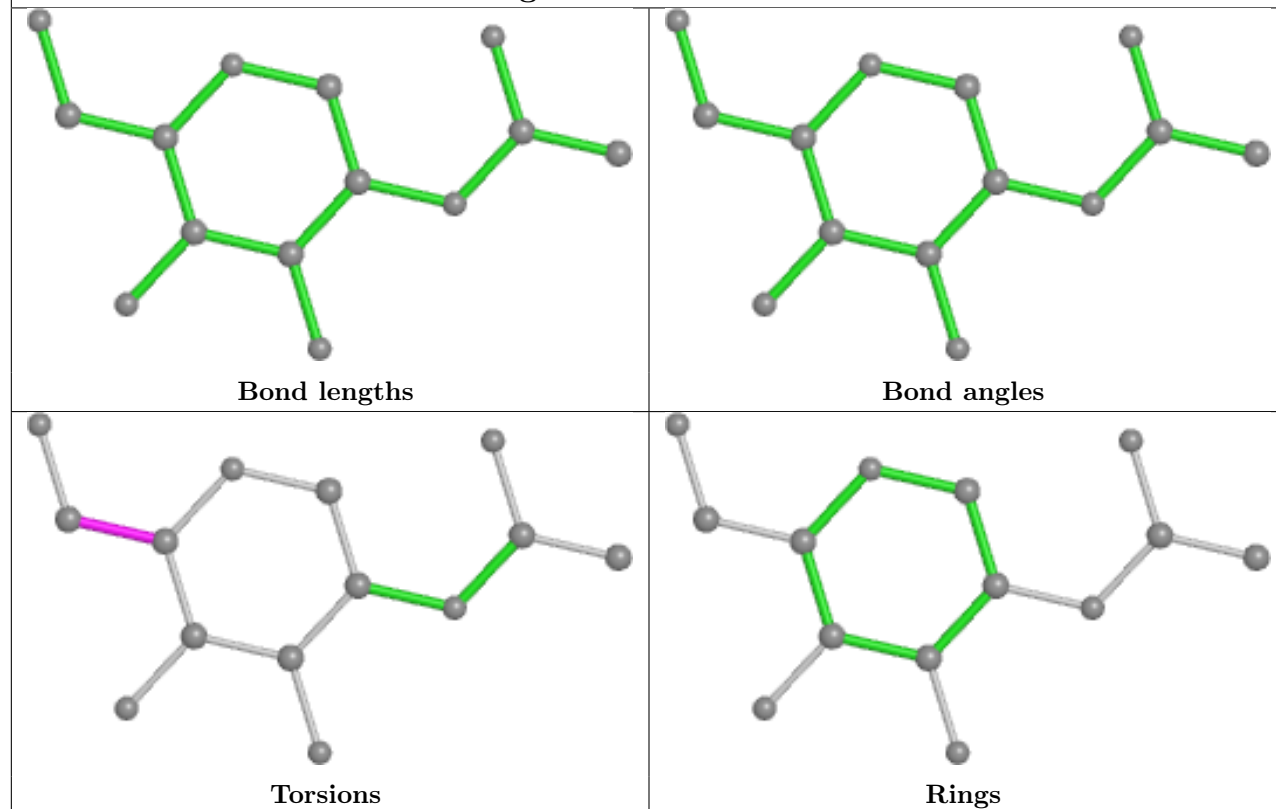
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

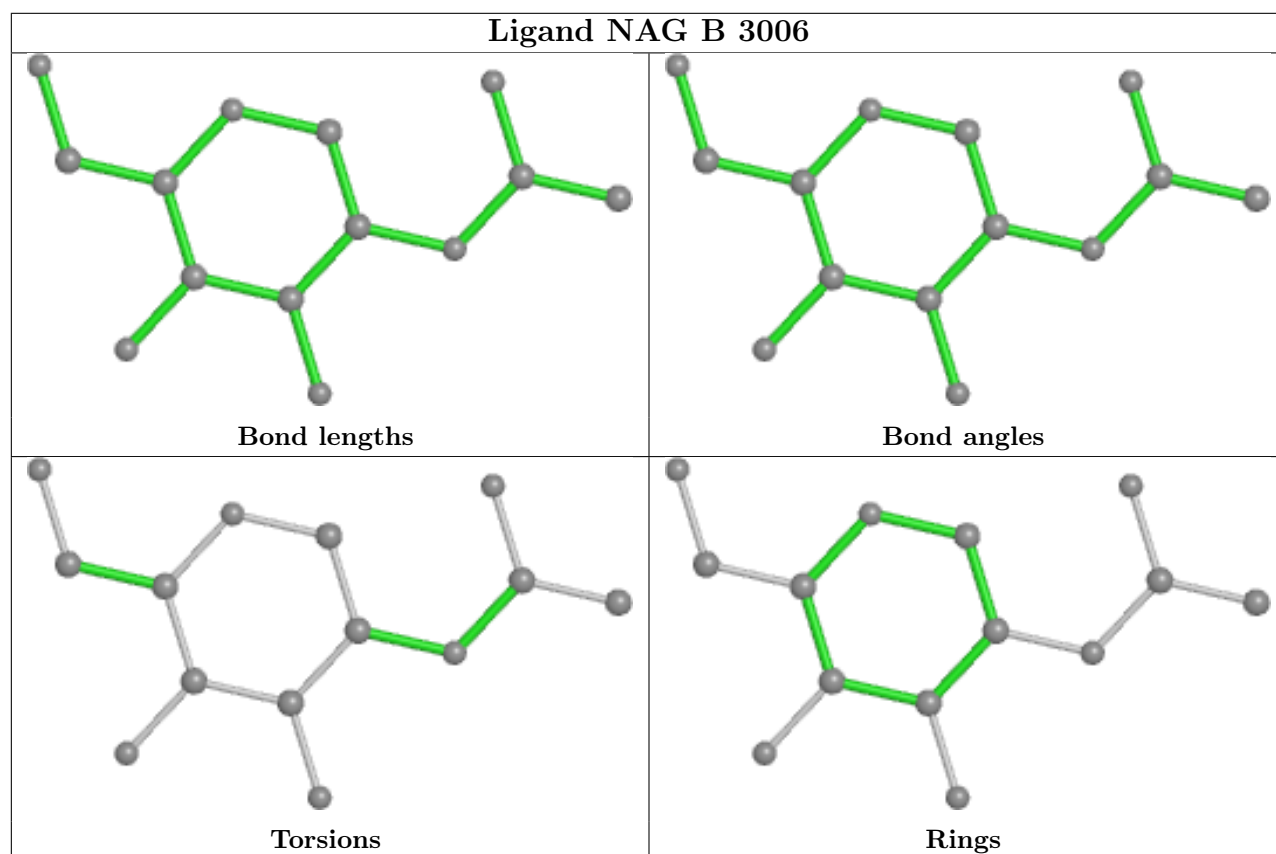
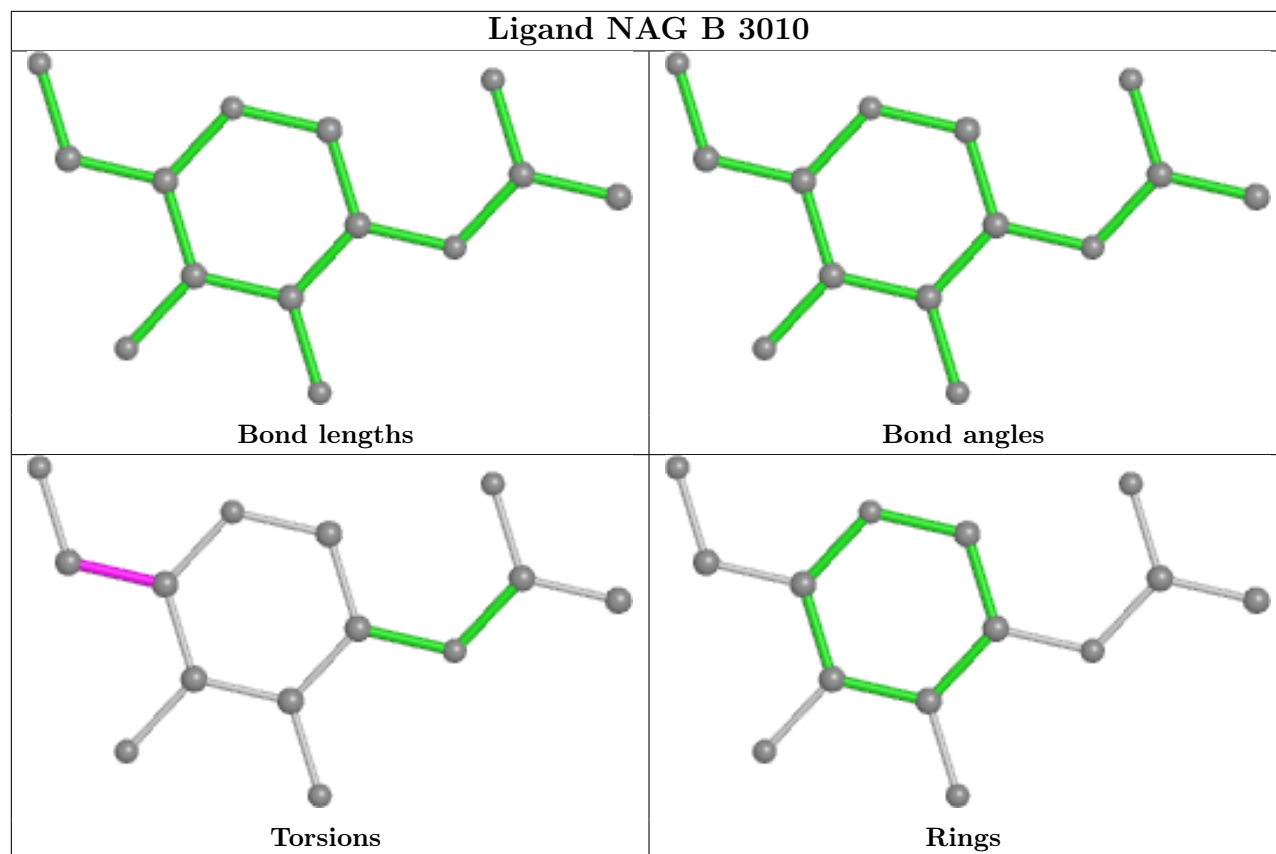


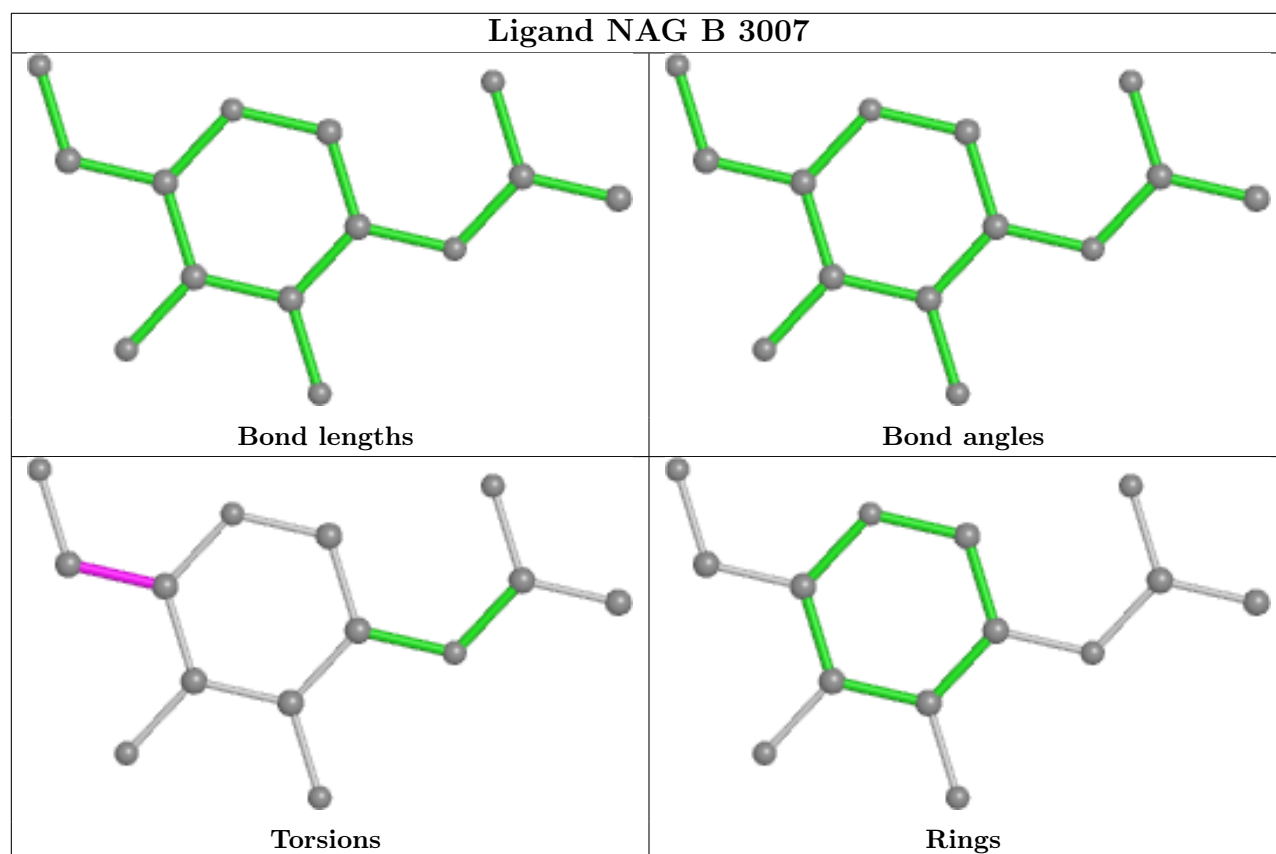
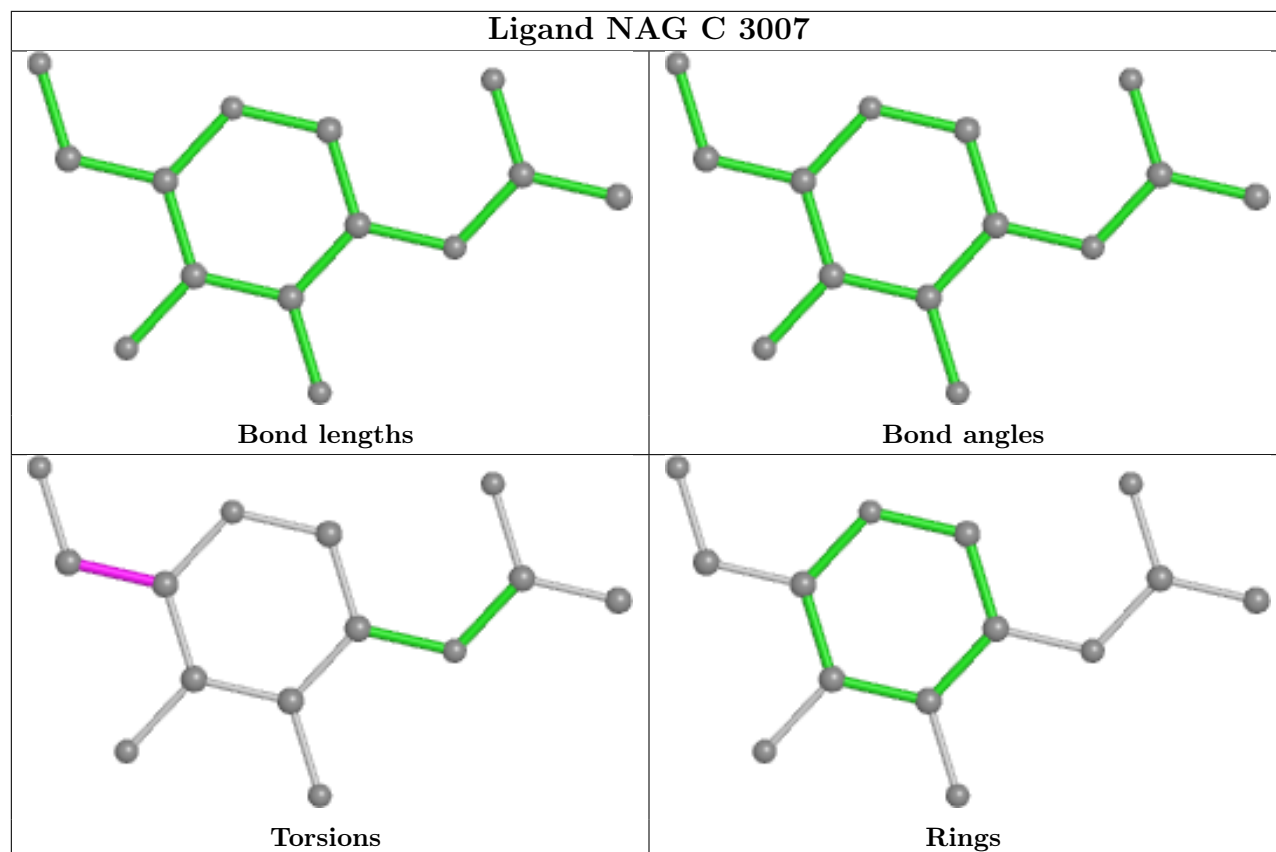
Ligand NAG A 3005



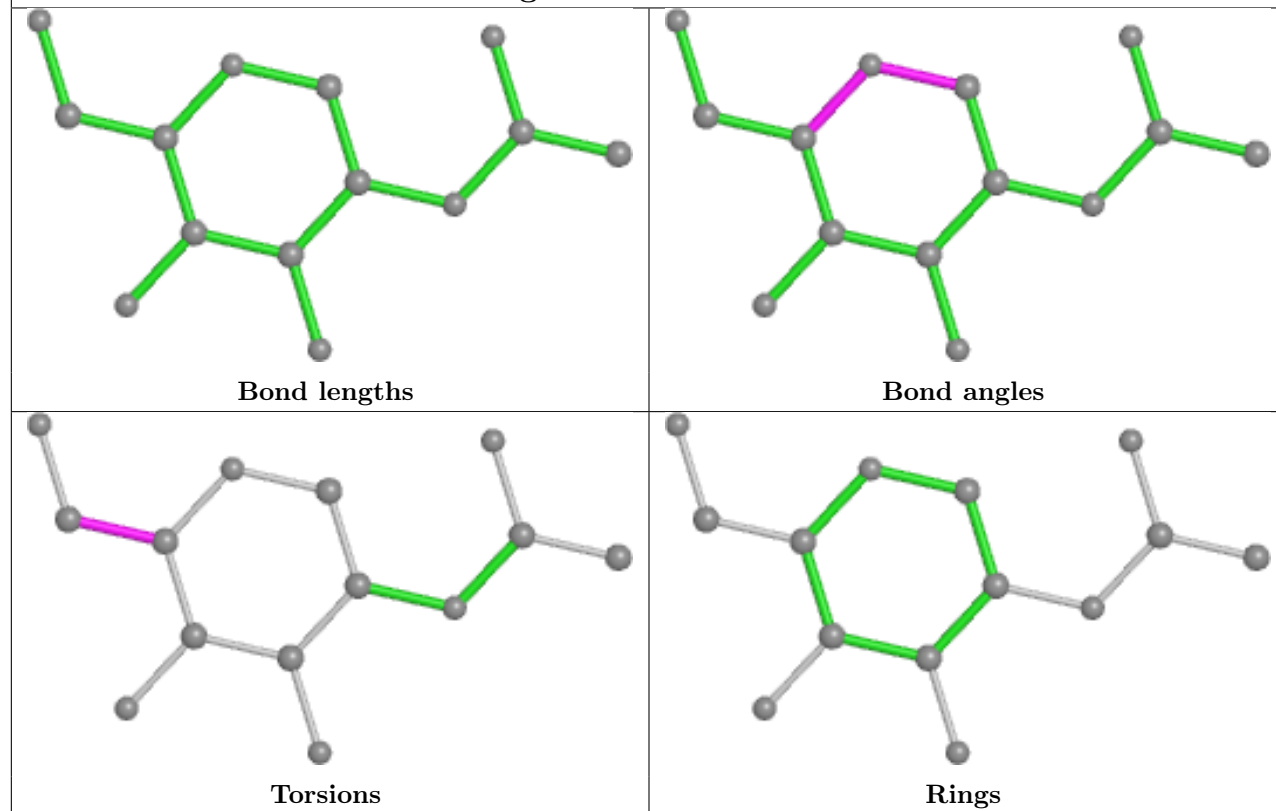
Ligand NAG C 3008



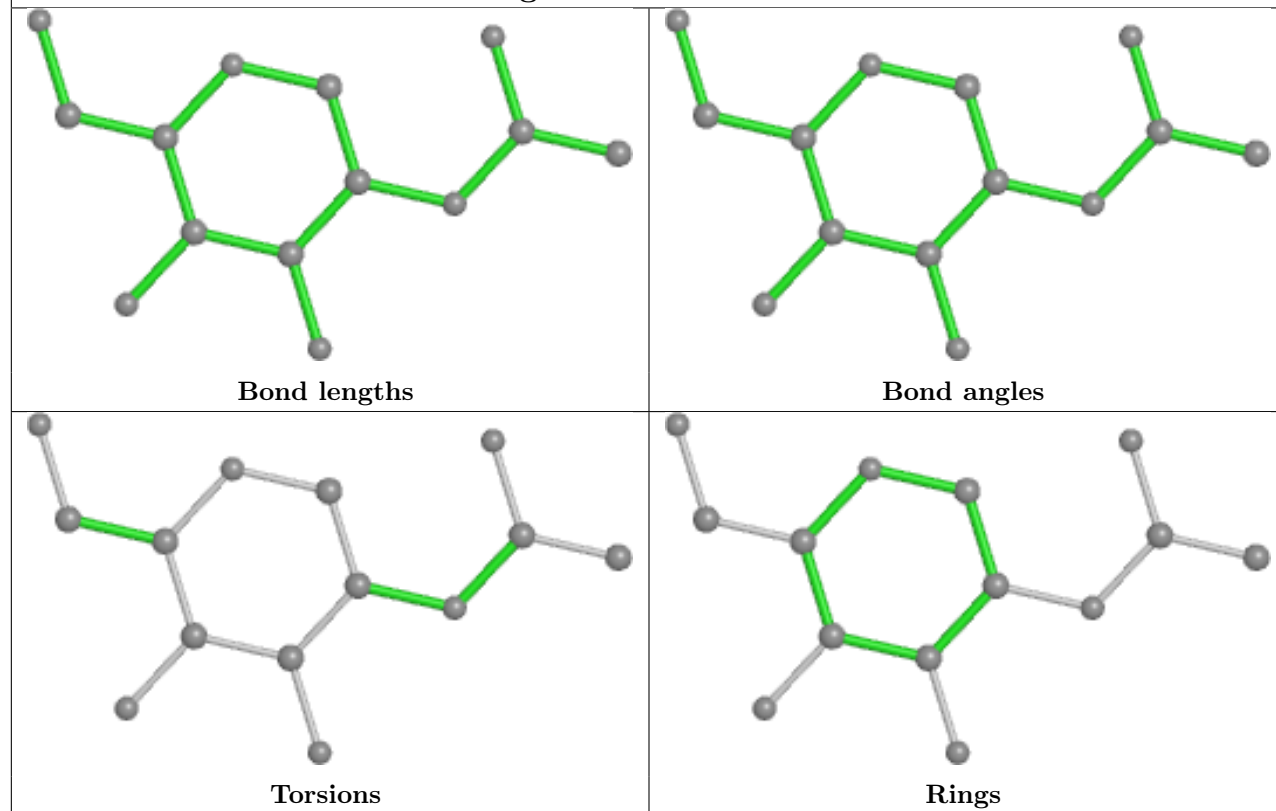


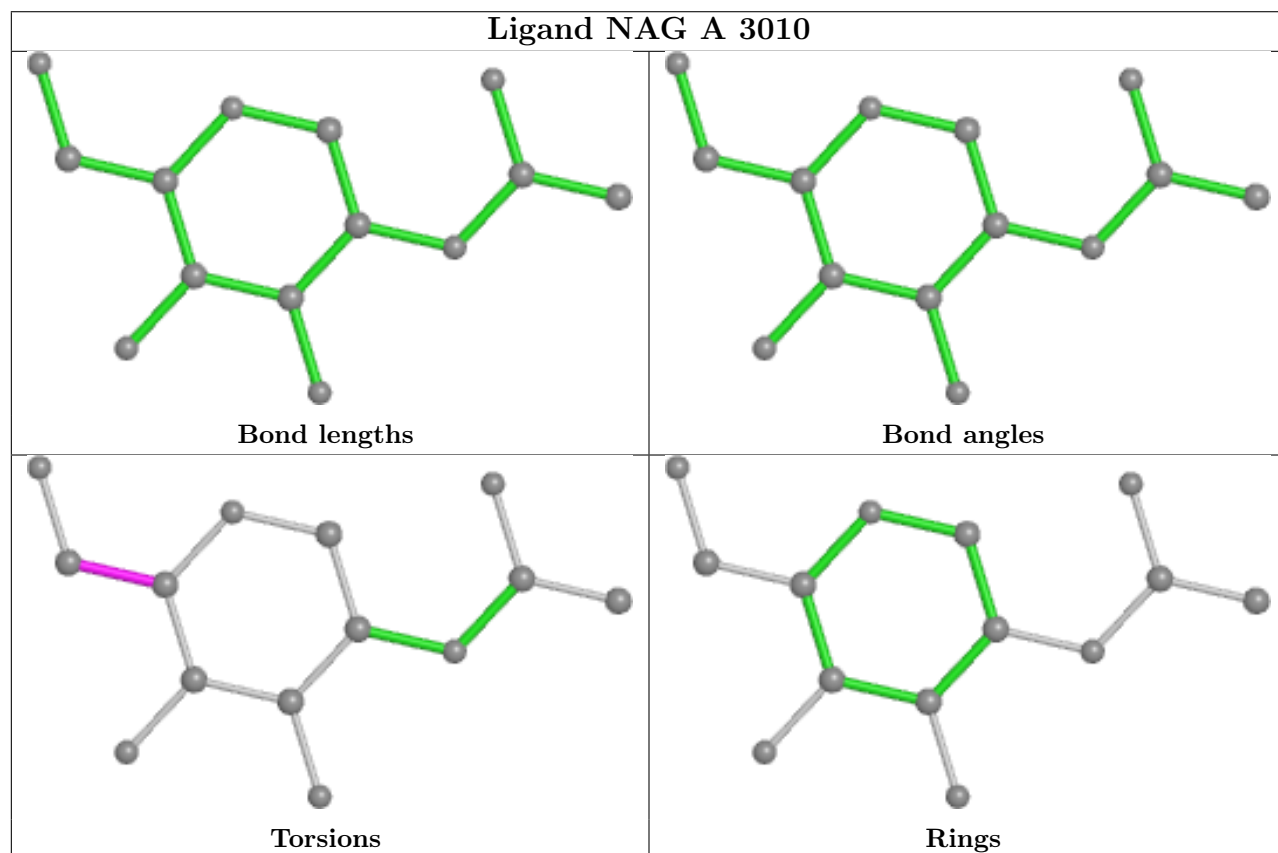
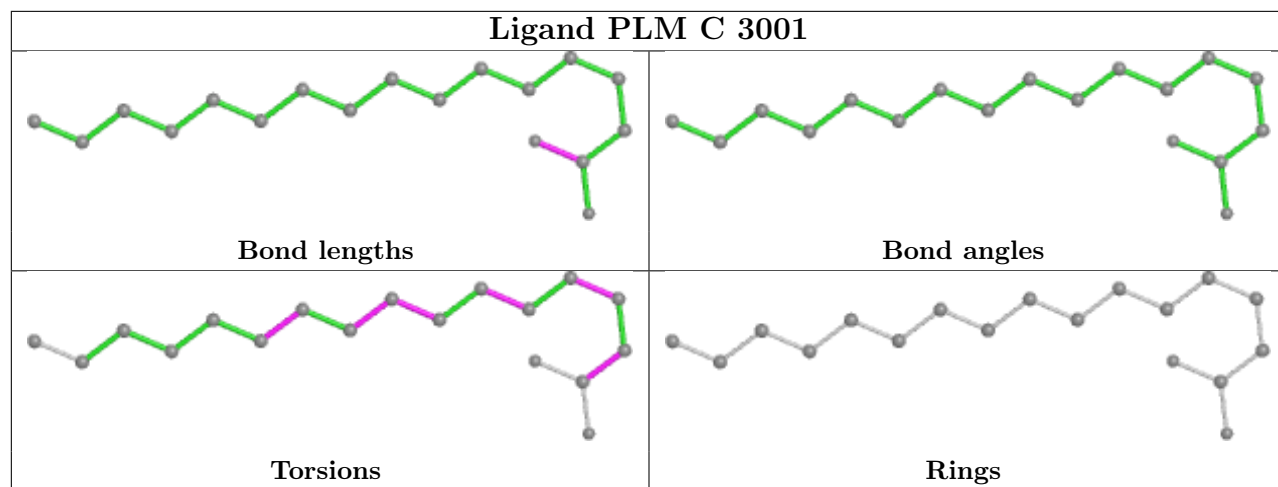


Ligand NAG B 3011

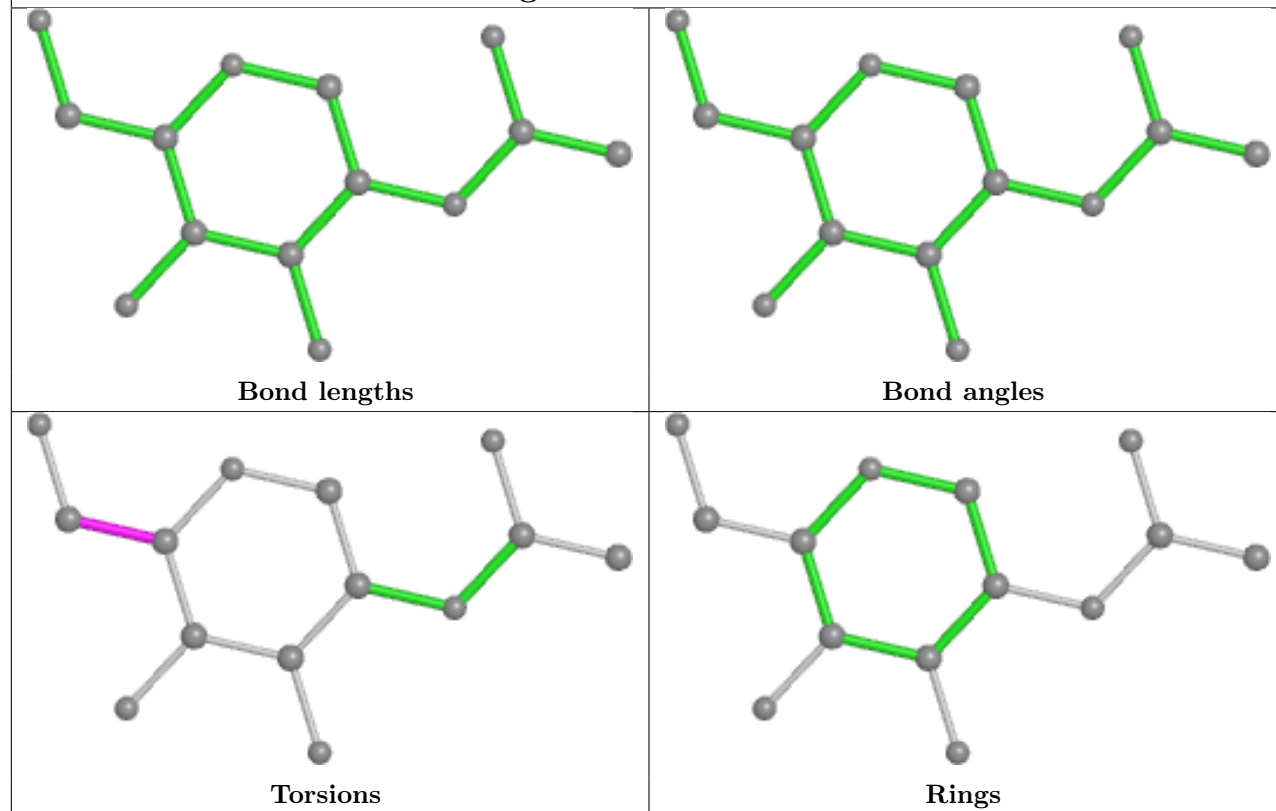


Ligand NAG B 3003

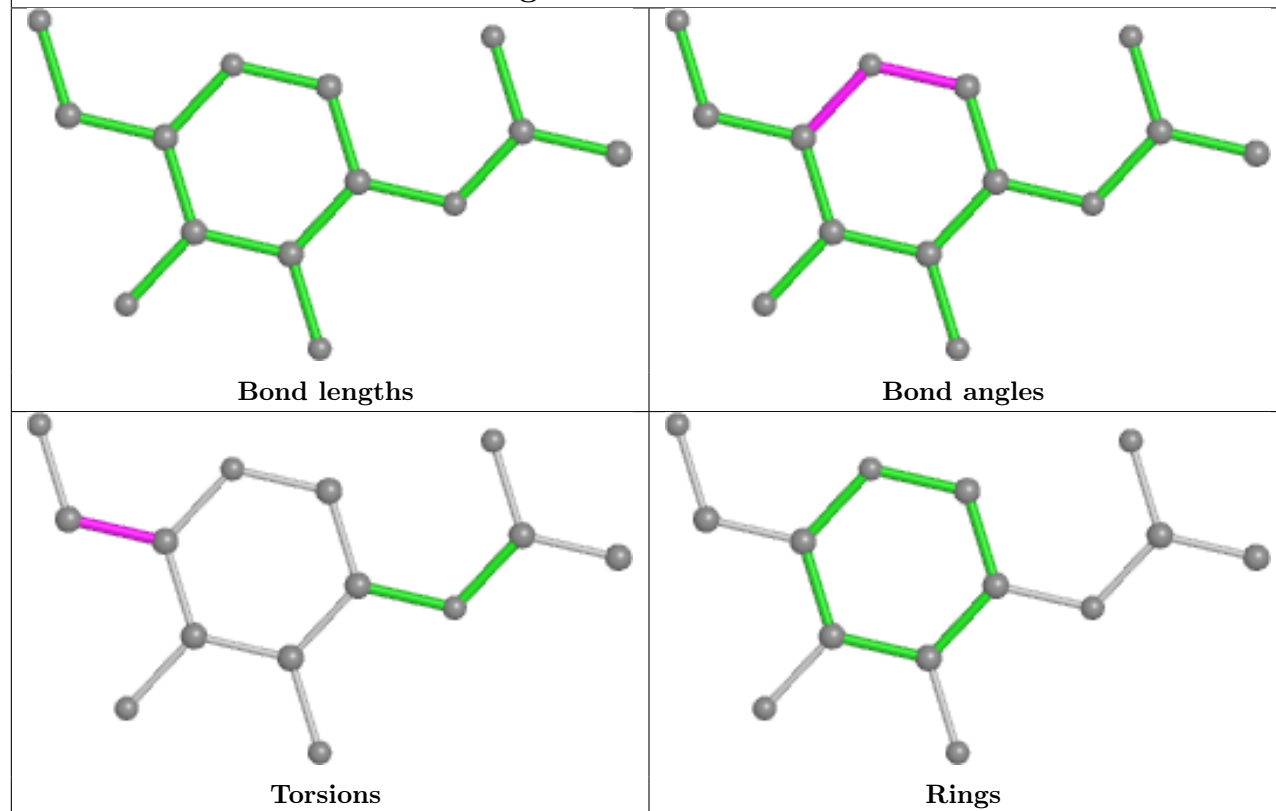


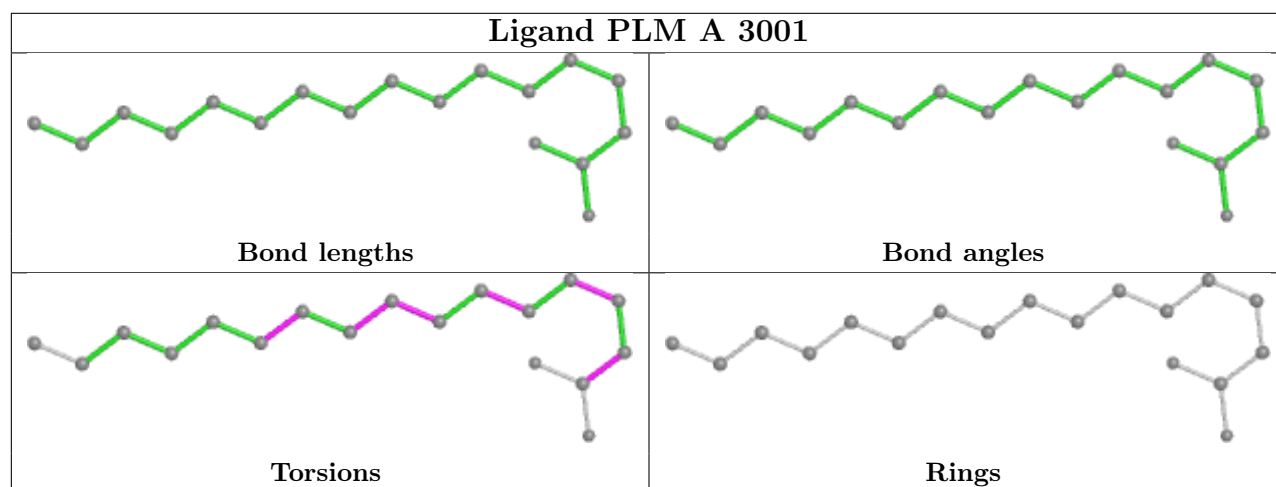
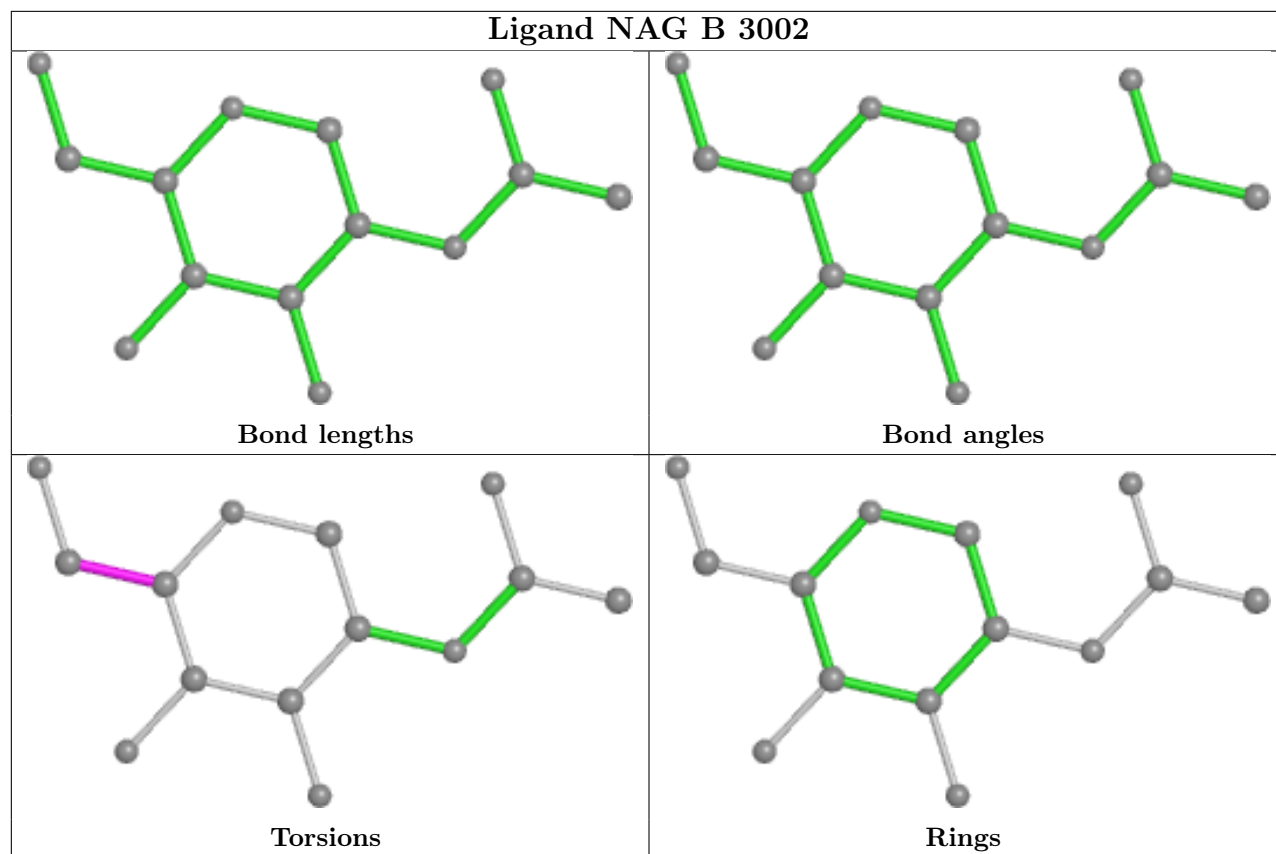


Ligand NAG B 3009

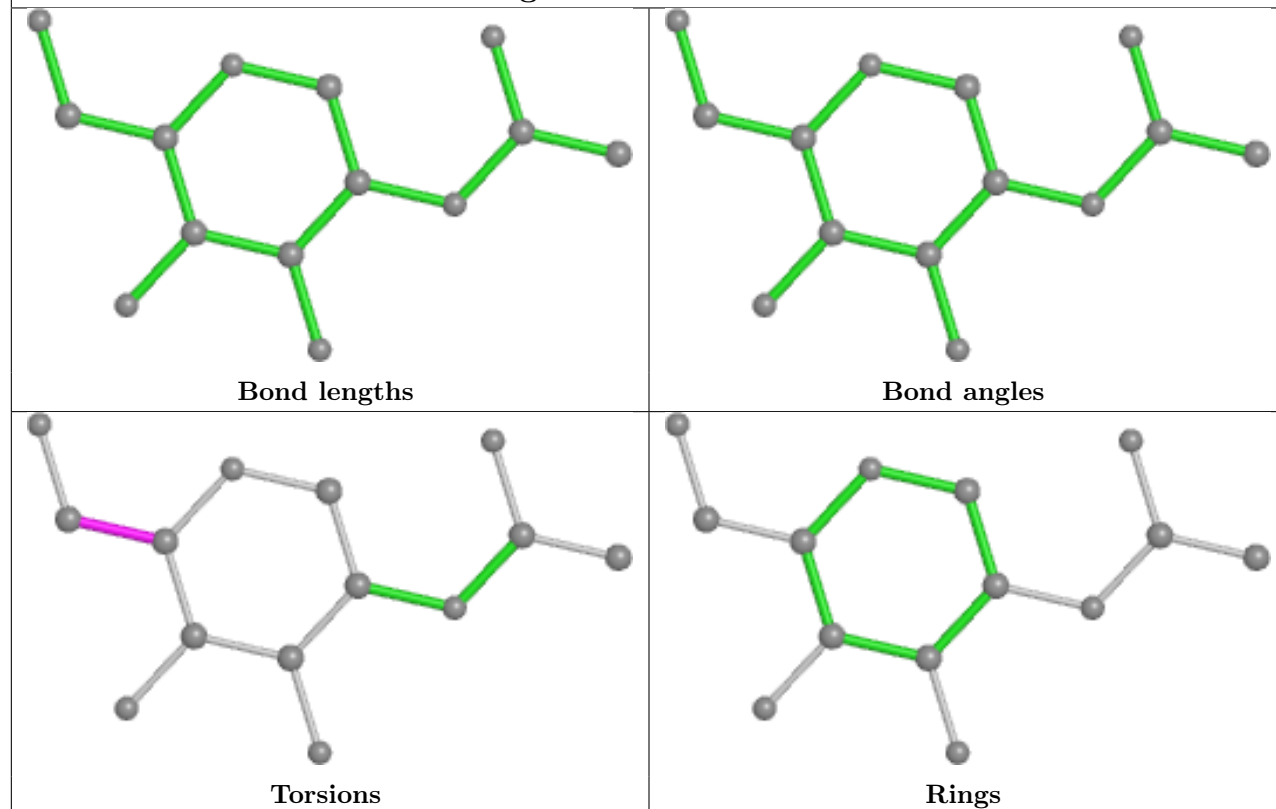


Ligand NAG B 3004

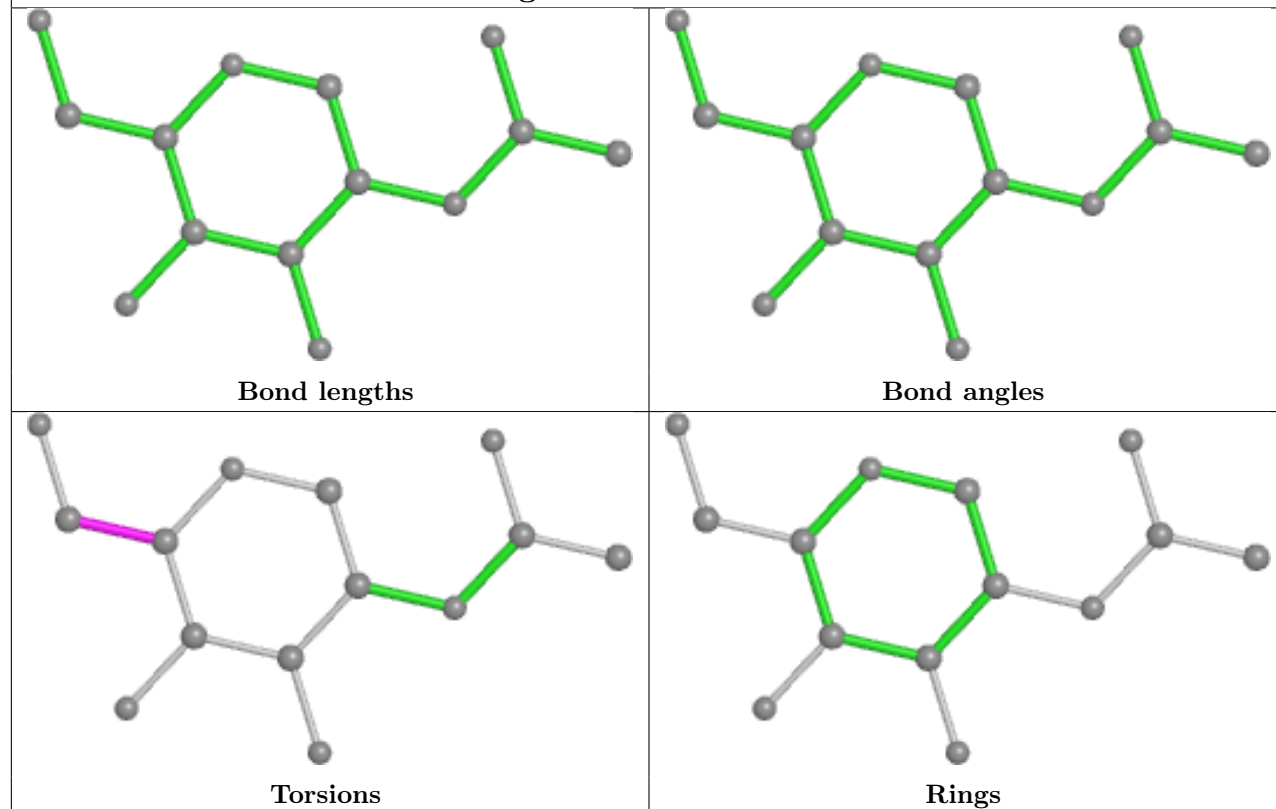




Ligand NAG B 3008



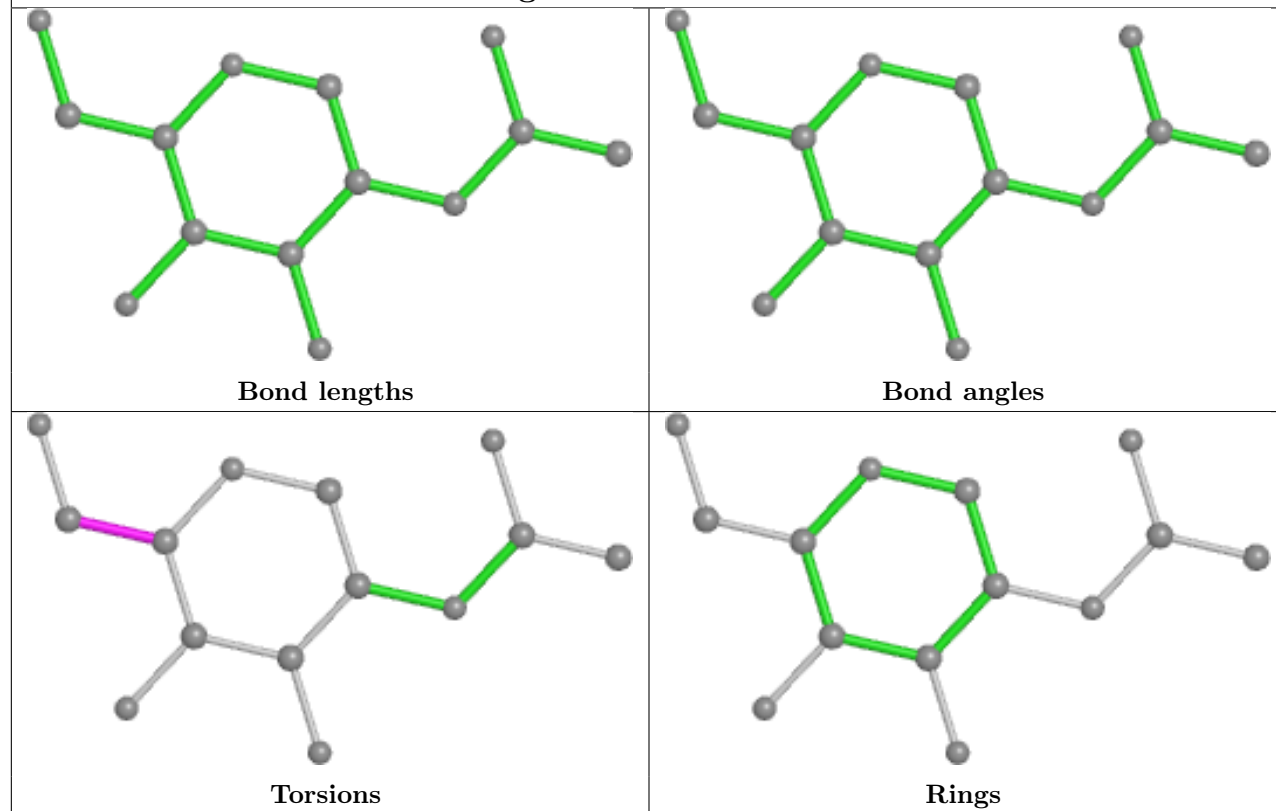
Ligand NAG A 3009

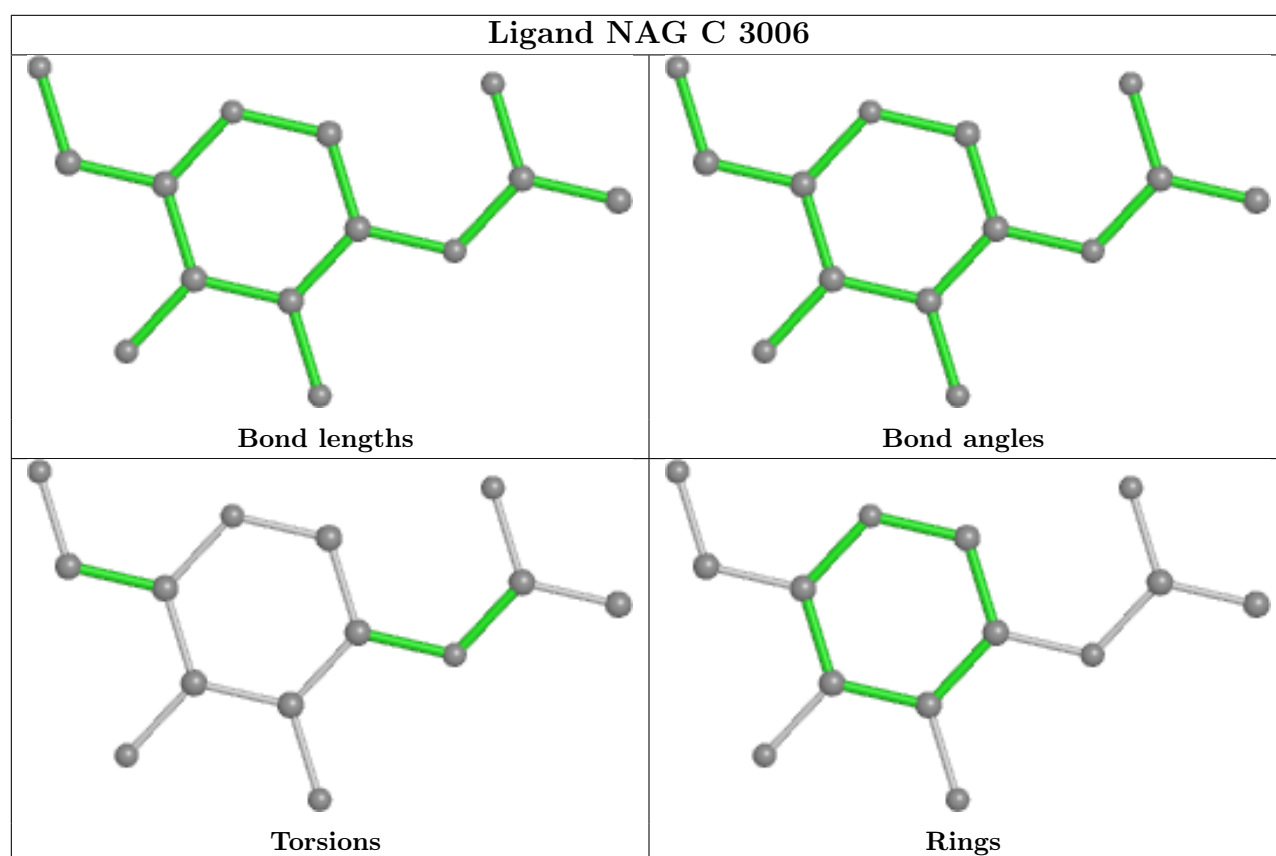
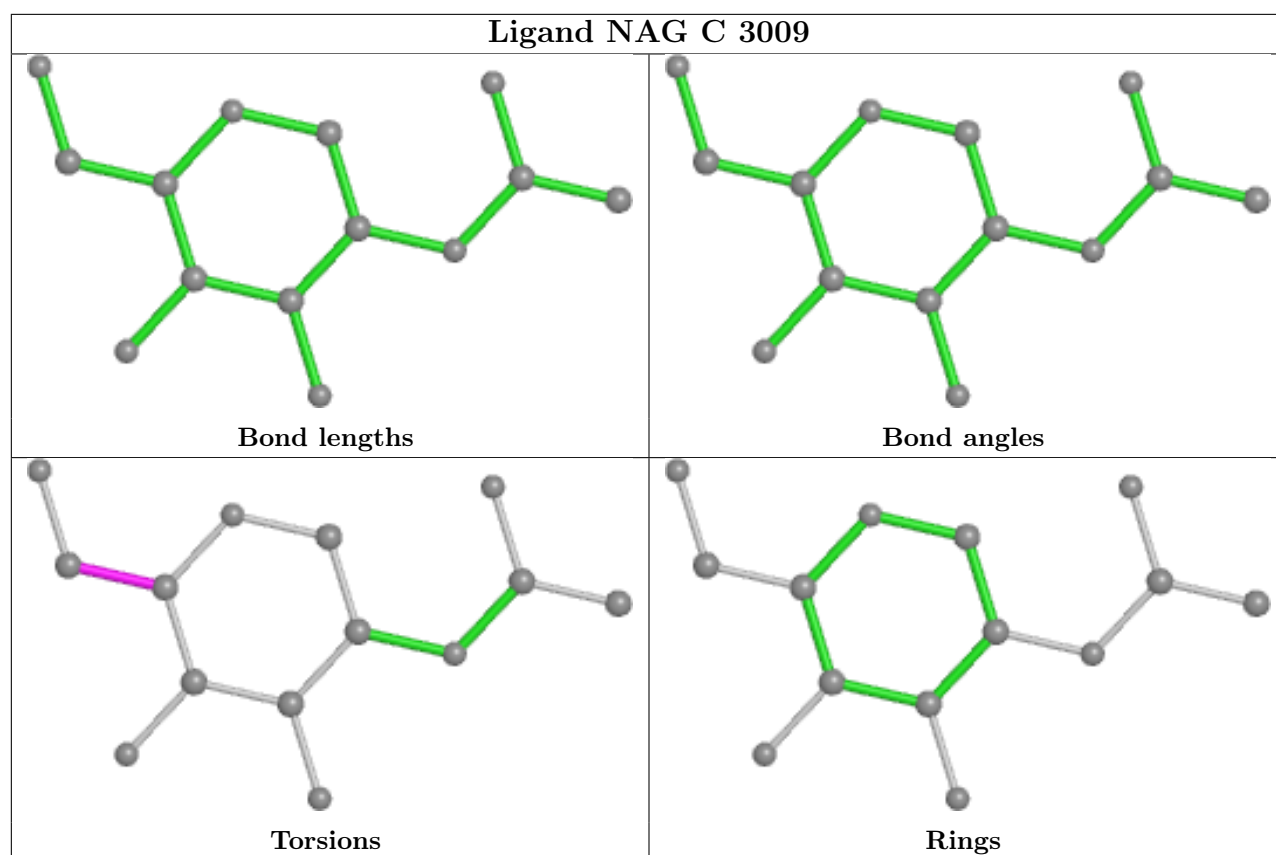


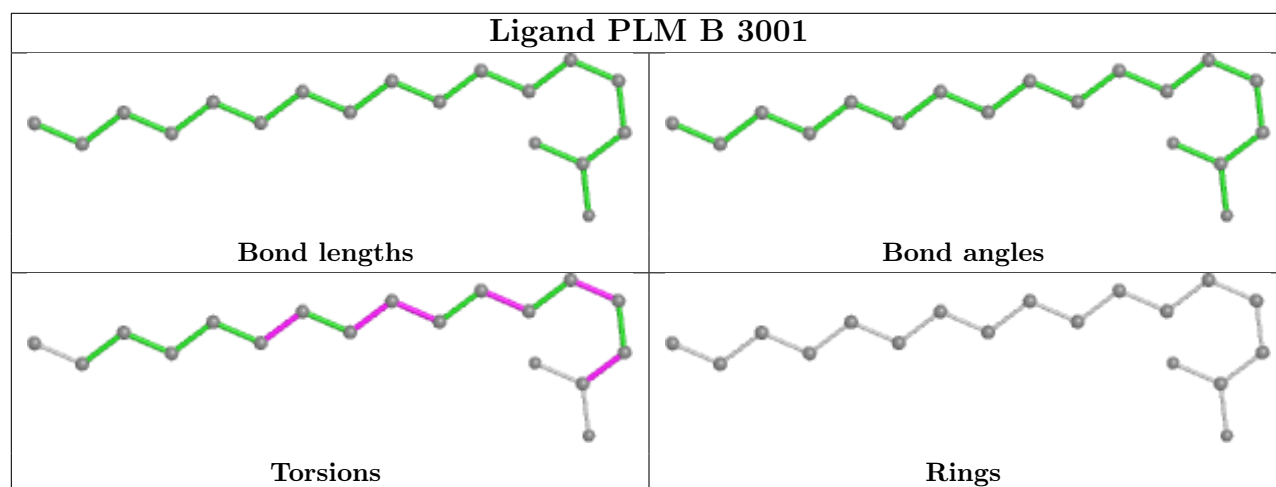
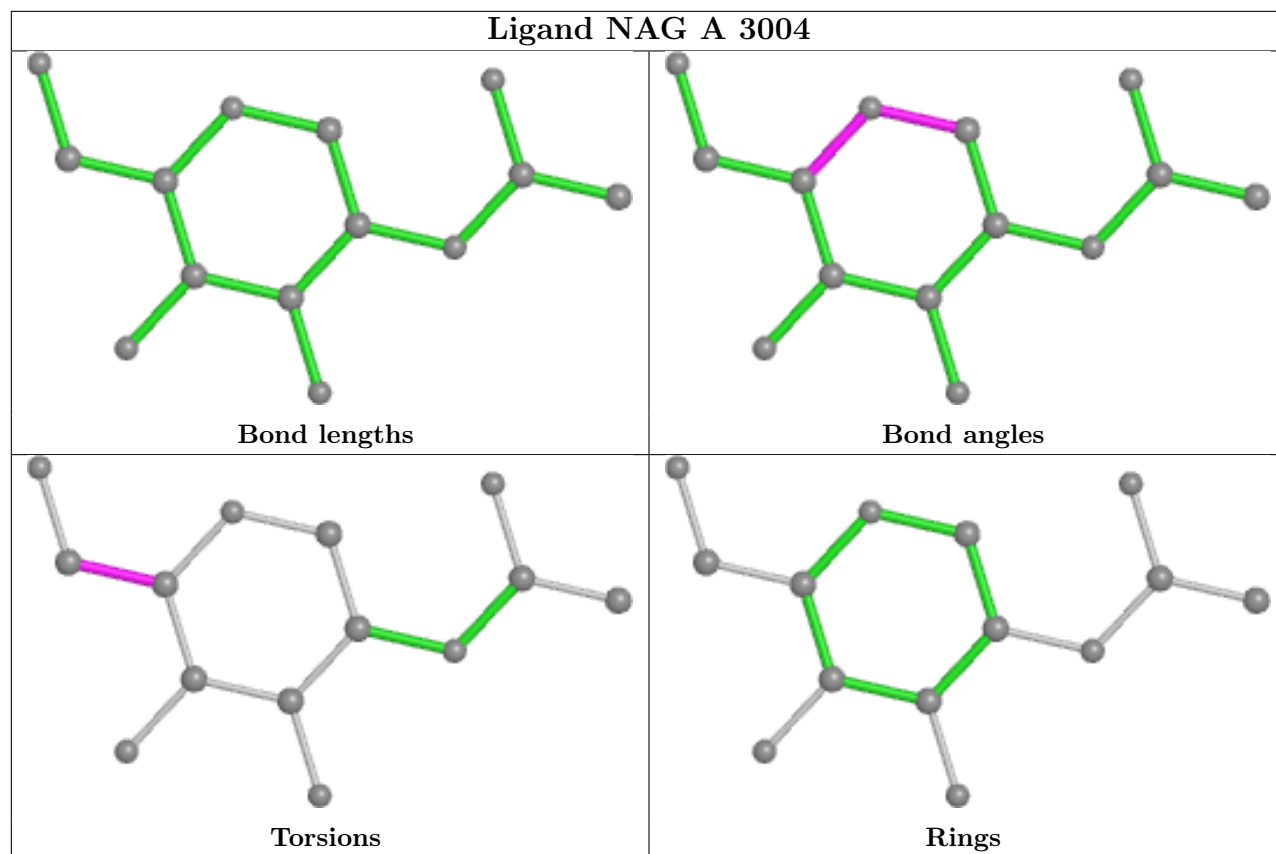
Ligand NAG C 3010



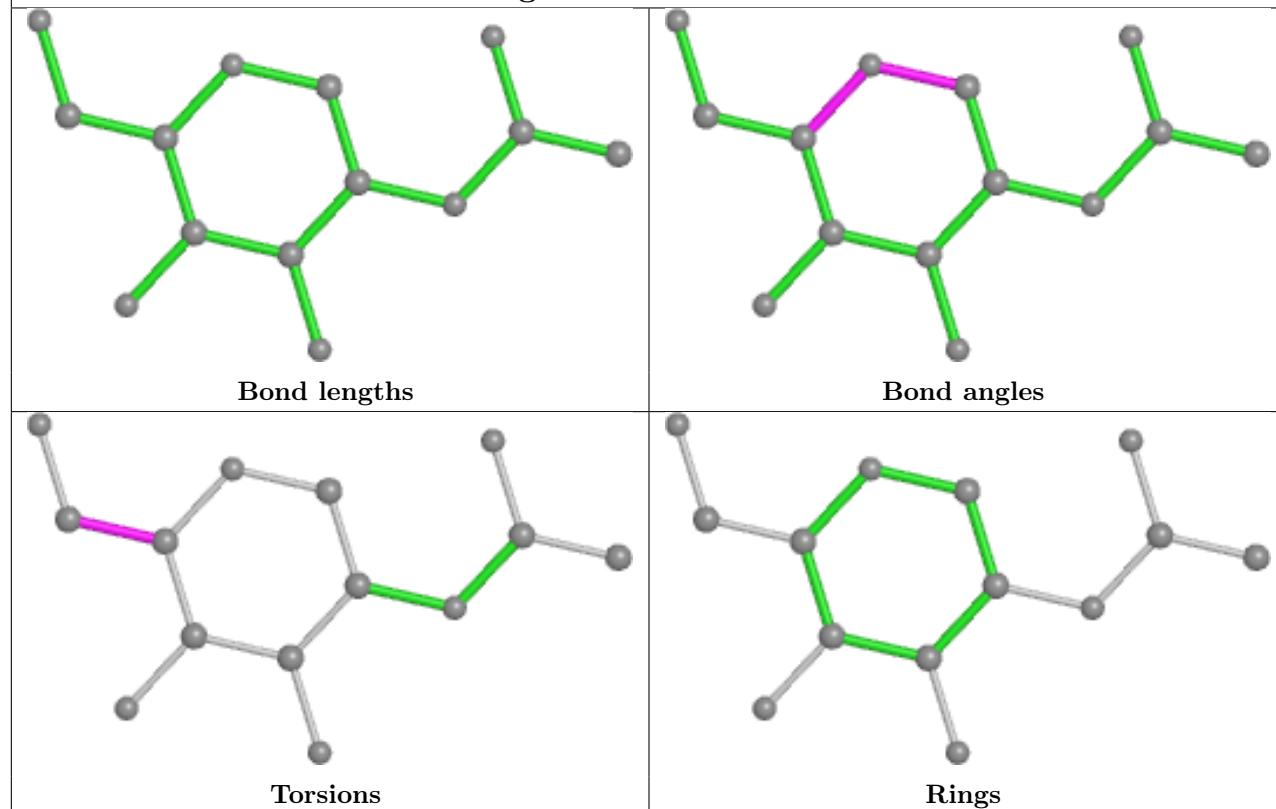
Ligand NAG A 3008



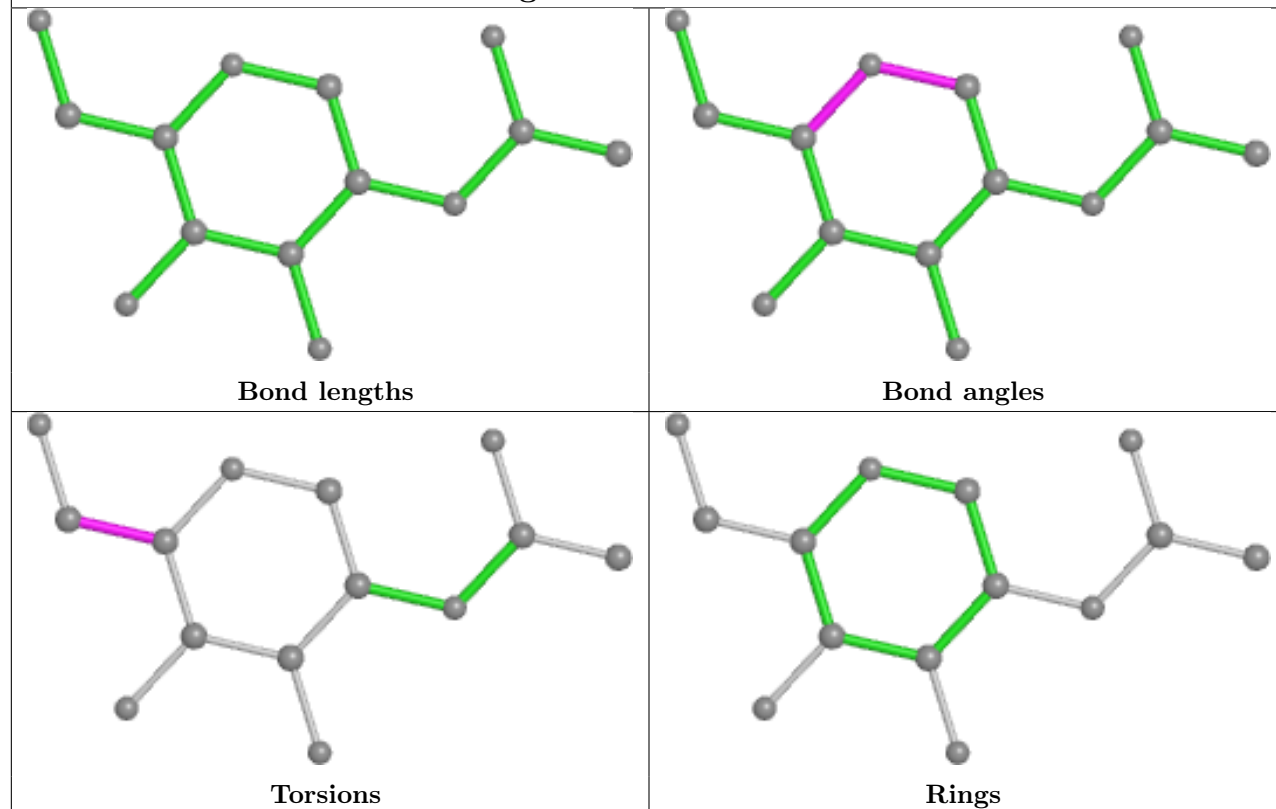




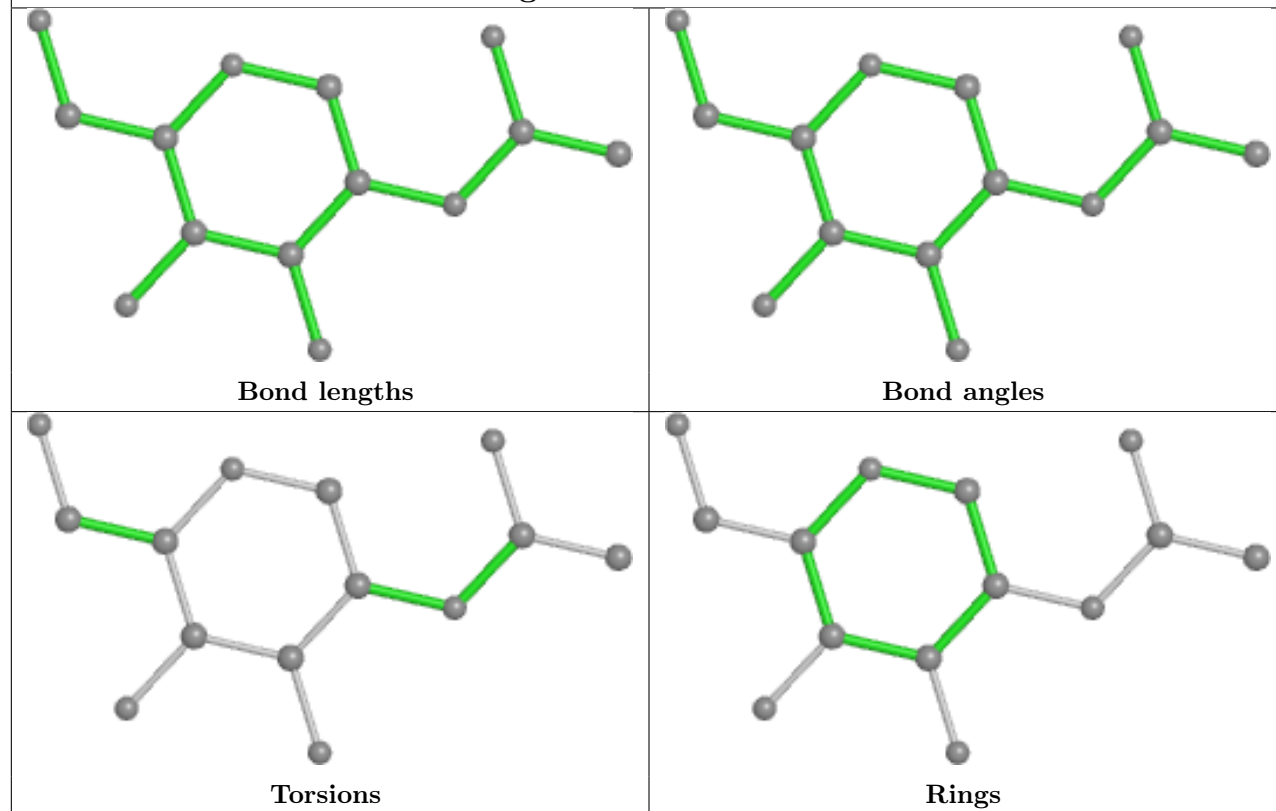
Ligand NAG A 3011



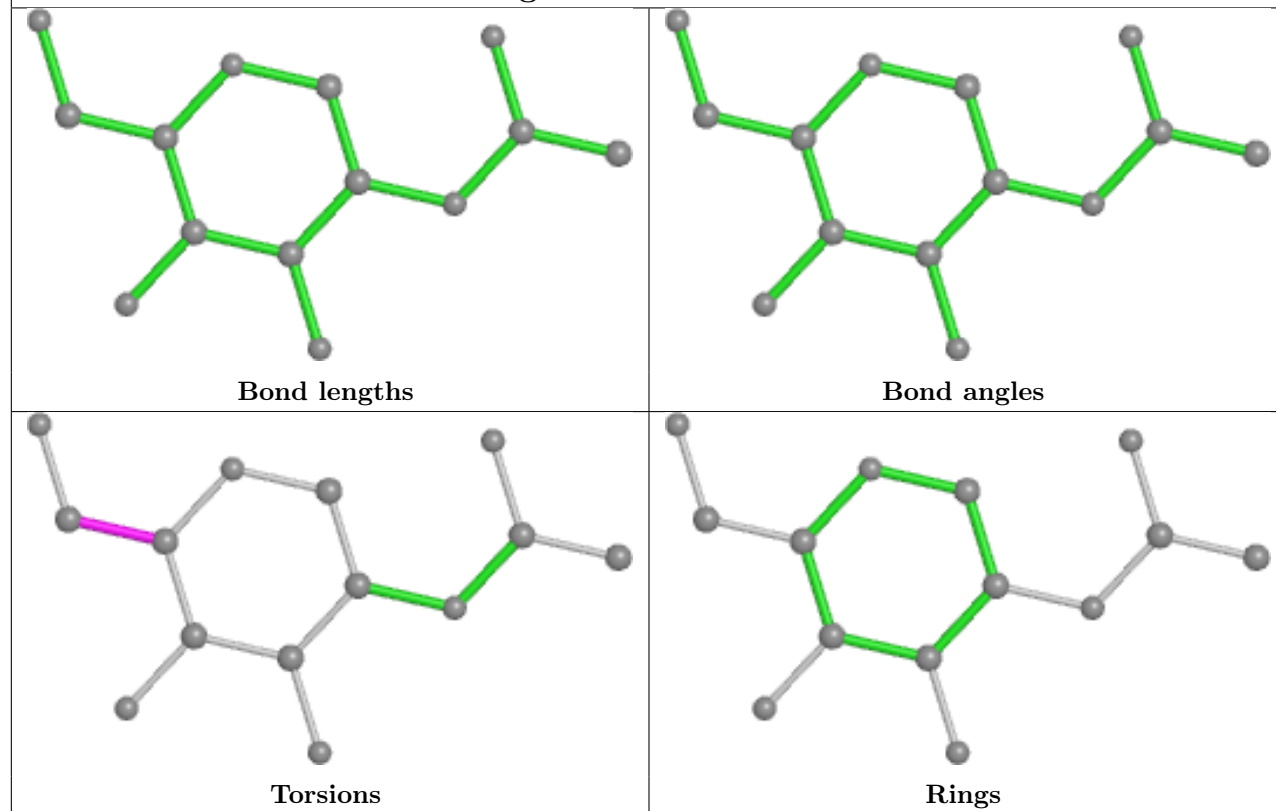
Ligand NAG C 3004



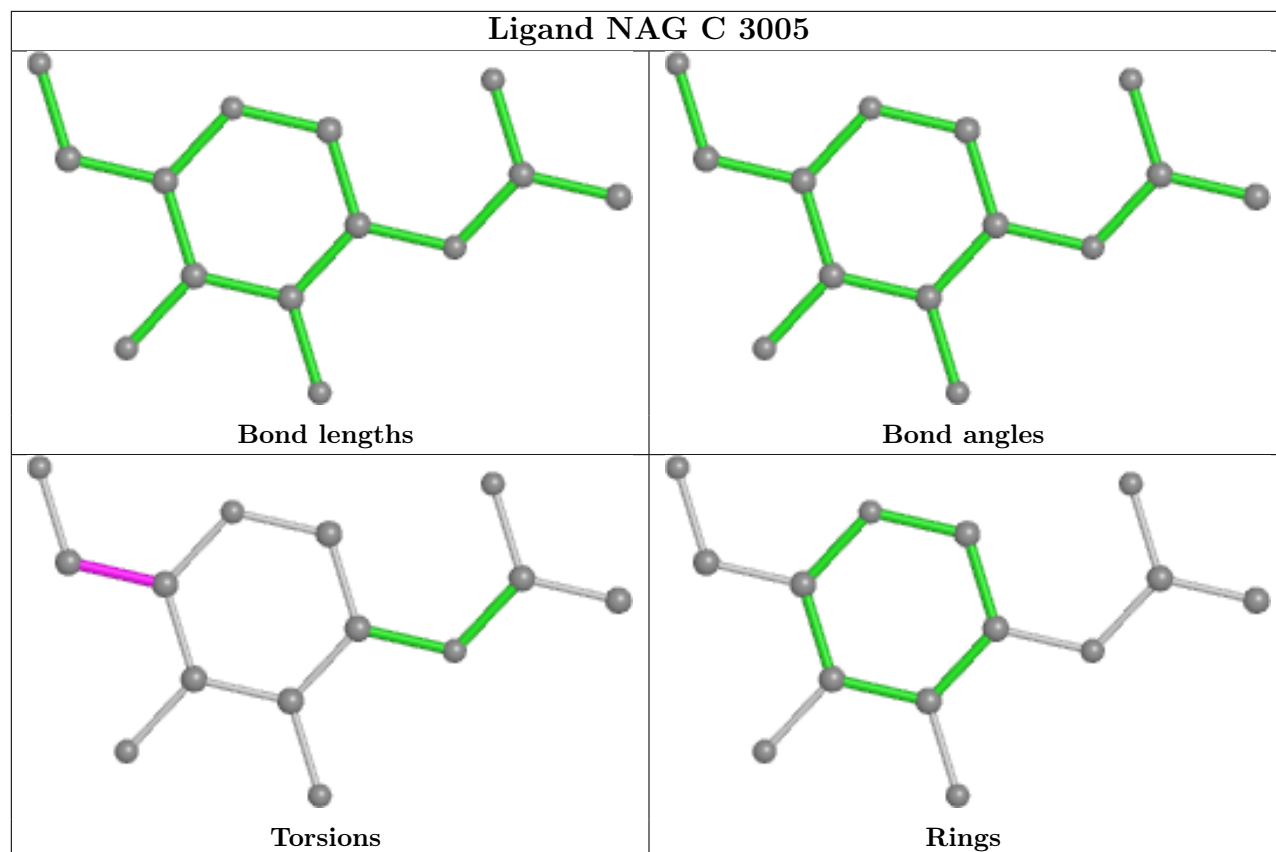
Ligand NAG C 3003



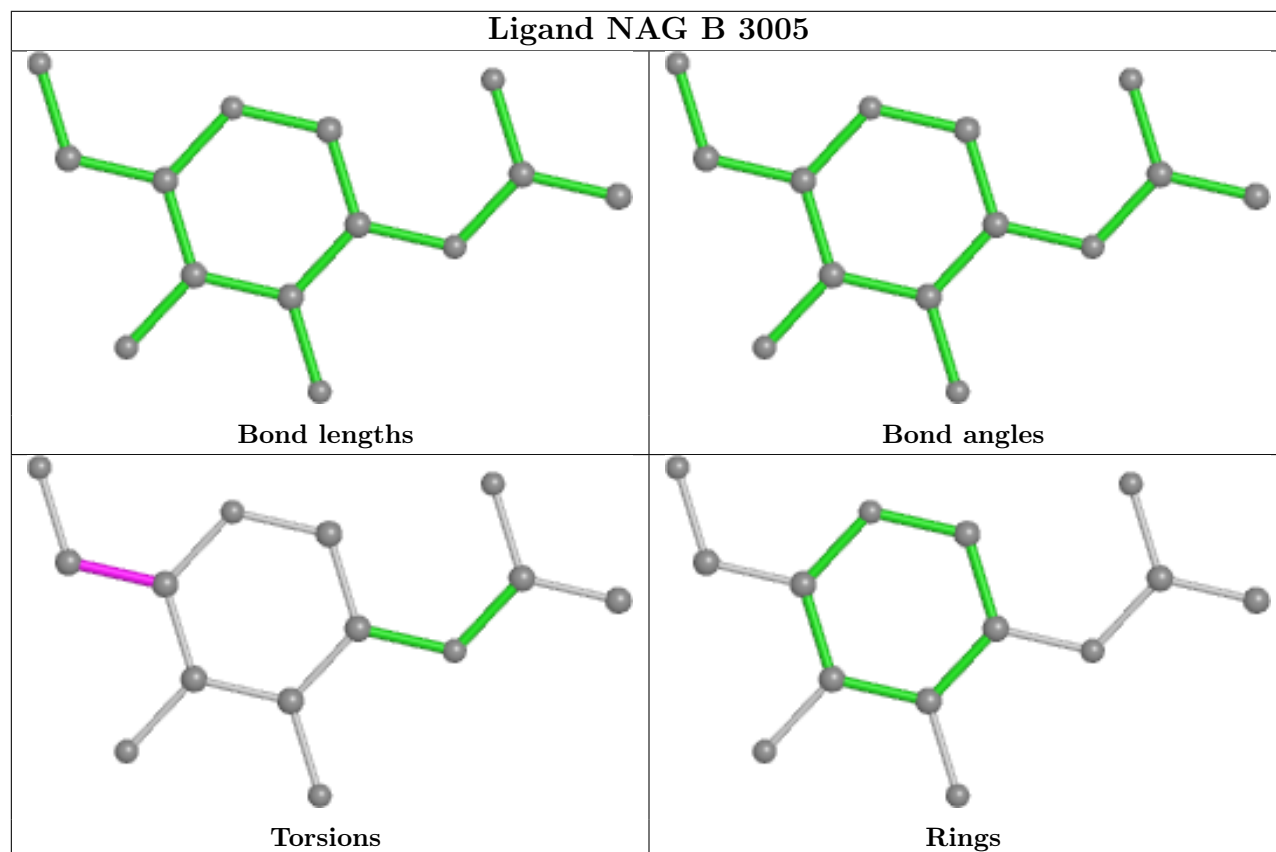
Ligand NAG C 3002

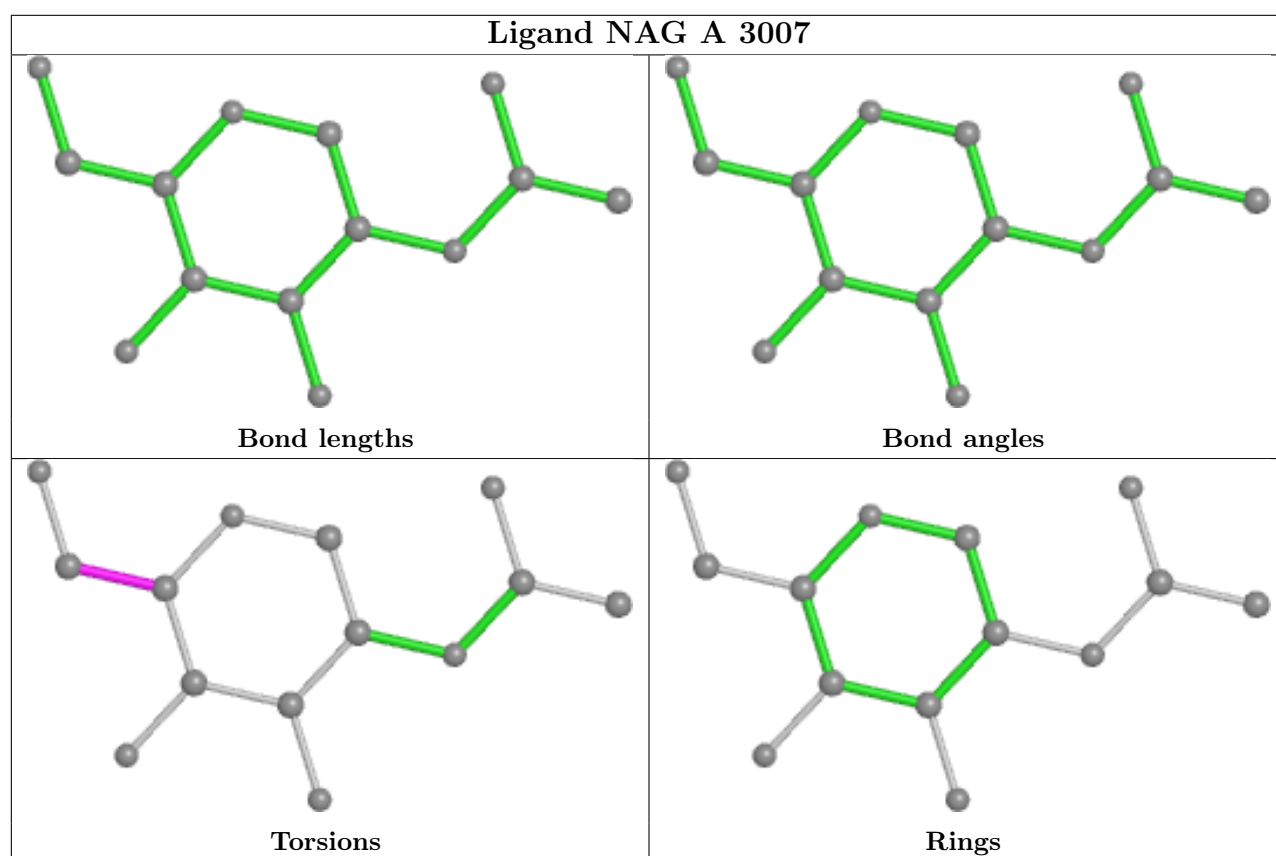
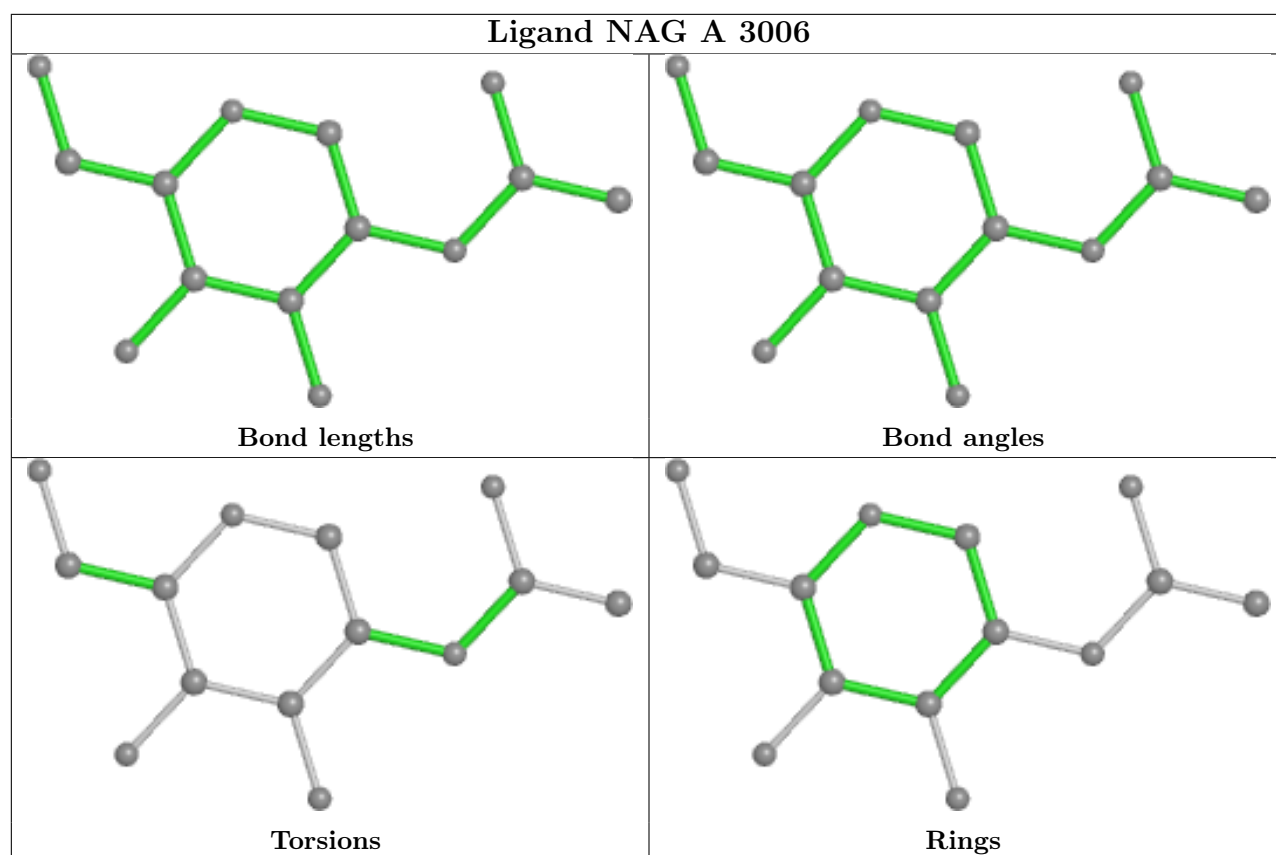


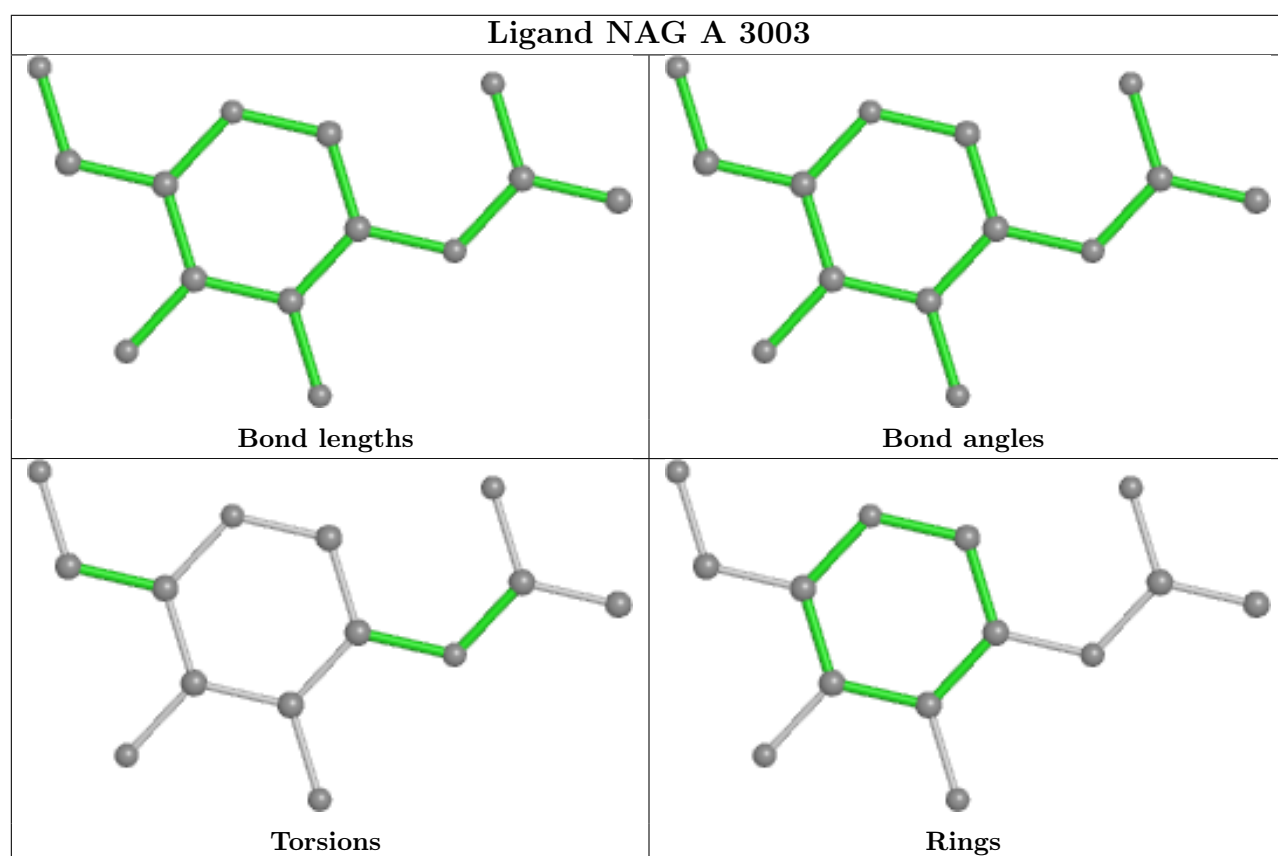
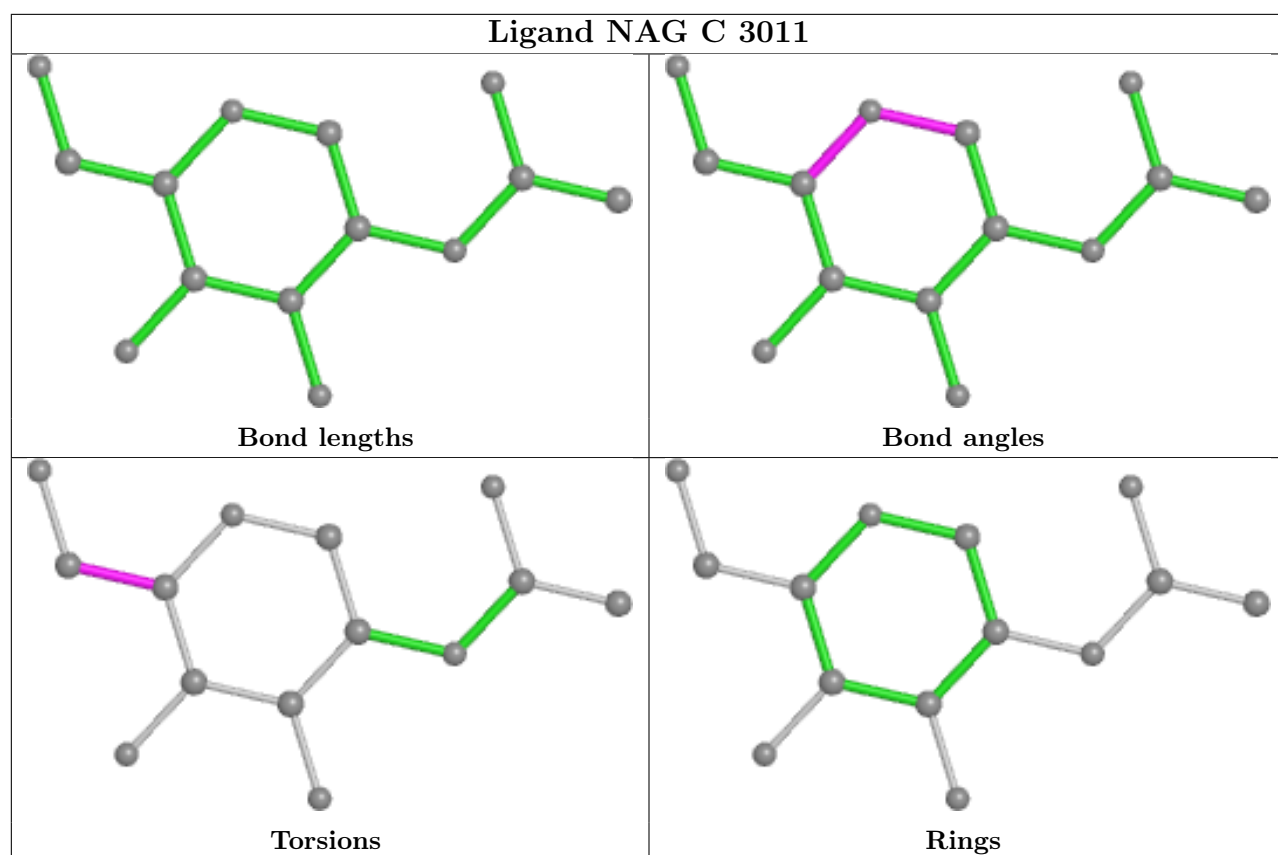
Ligand NAG C 3005



Ligand NAG B 3005







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

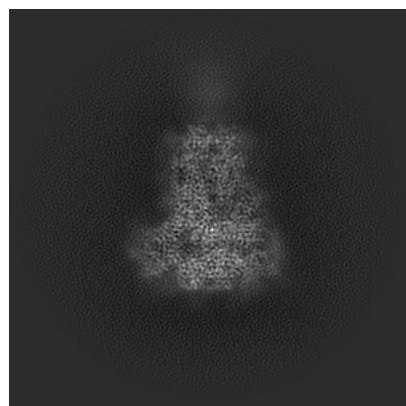
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62523. These allow visual inspection of the internal detail of the map and identification of artifacts.

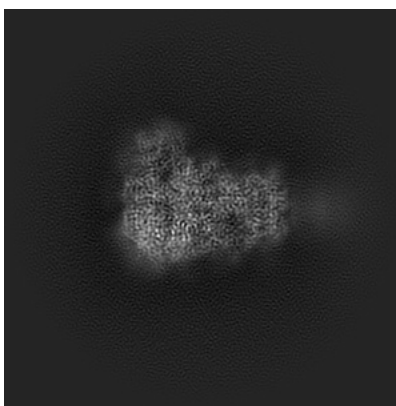
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

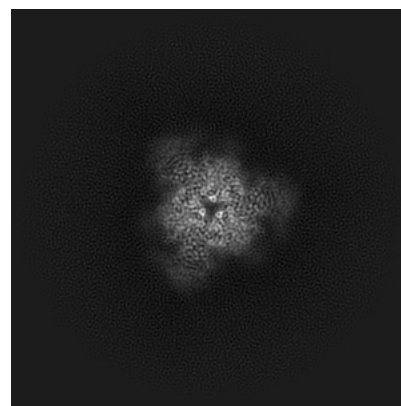
6.1.1 Primary map



X

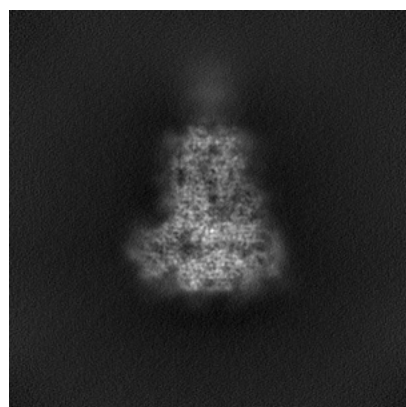


Y

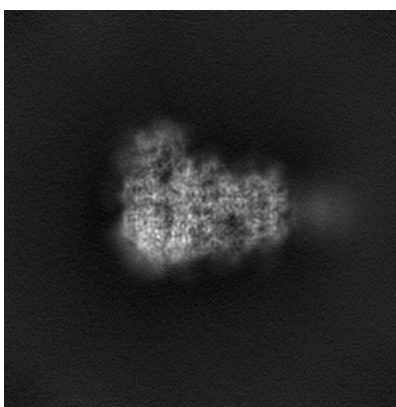


Z

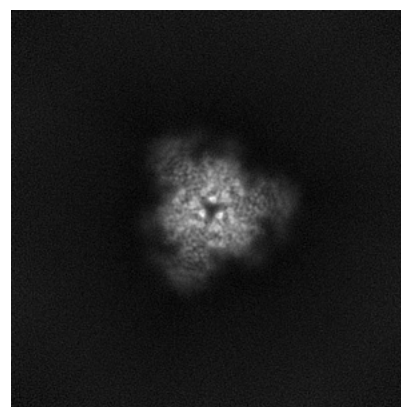
6.1.2 Raw map



X



Y

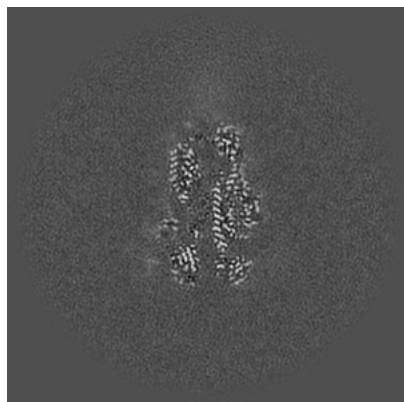


Z

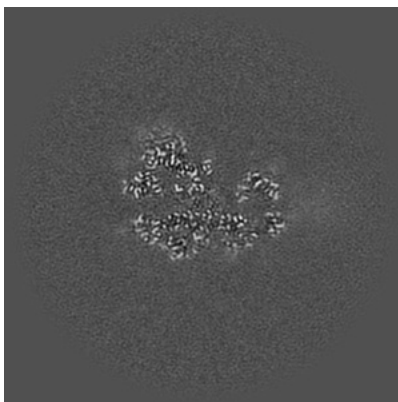
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

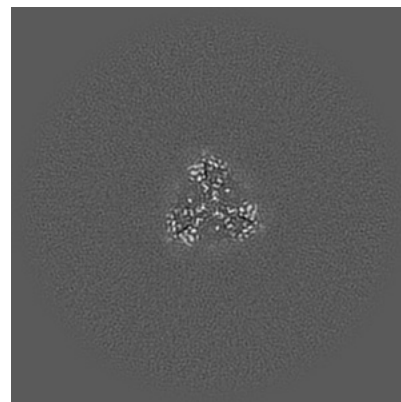
6.2.1 Primary map



X Index: 160

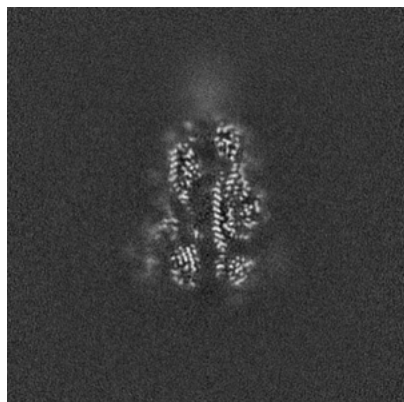


Y Index: 160

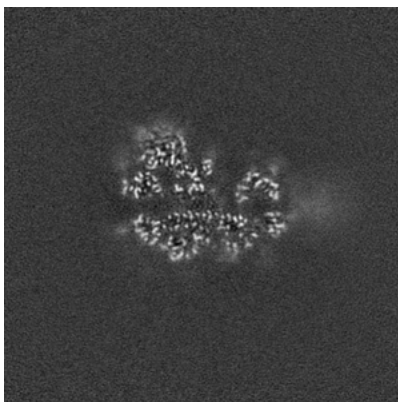


Z Index: 160

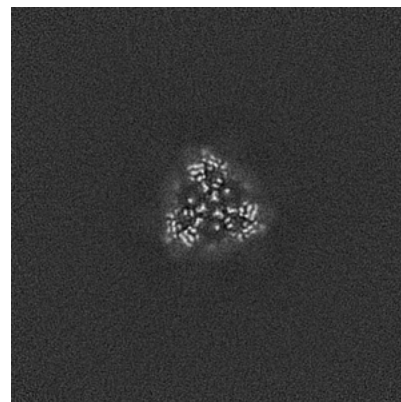
6.2.2 Raw map



X Index: 160



Y Index: 160

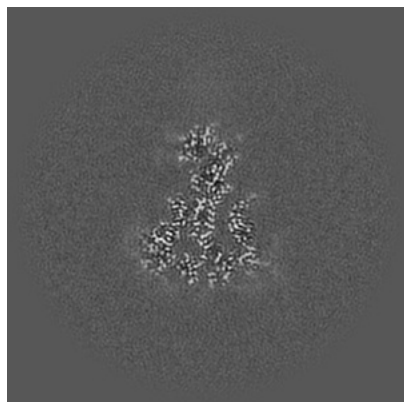


Z Index: 160

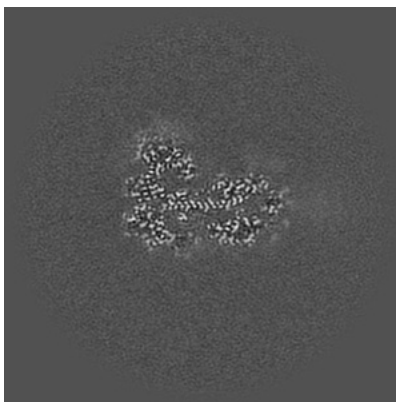
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

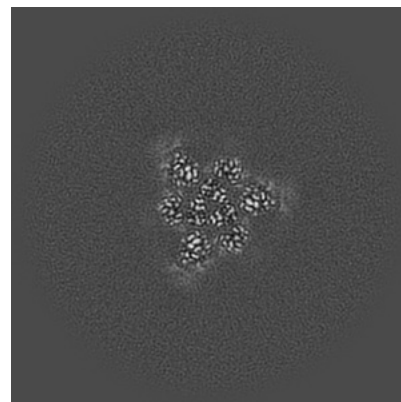
6.3.1 Primary map



X Index: 144

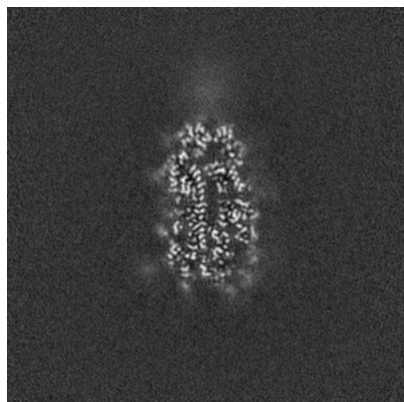


Y Index: 168

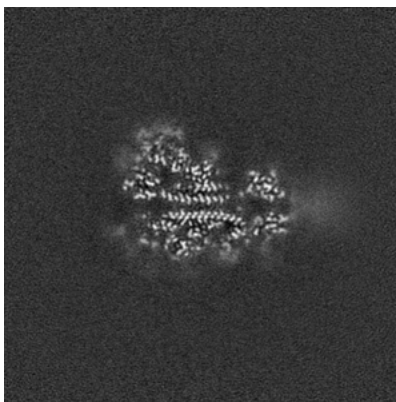


Z Index: 139

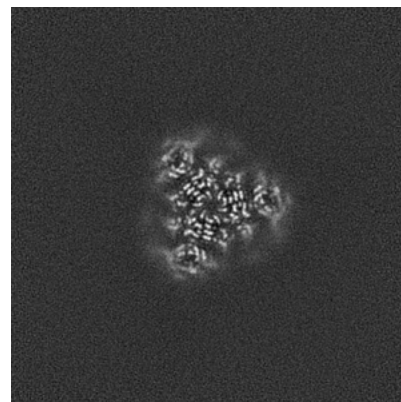
6.3.2 Raw map



X Index: 168



Y Index: 157

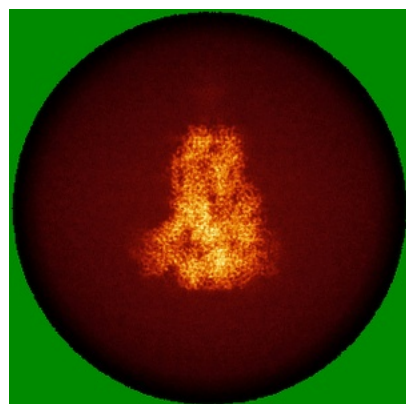


Z Index: 115

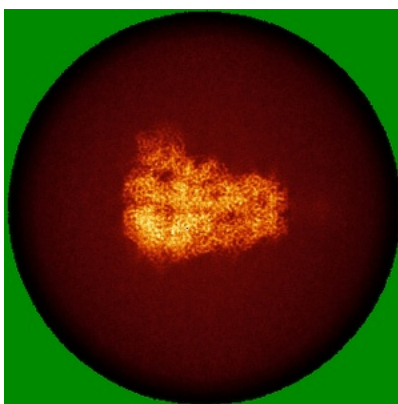
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

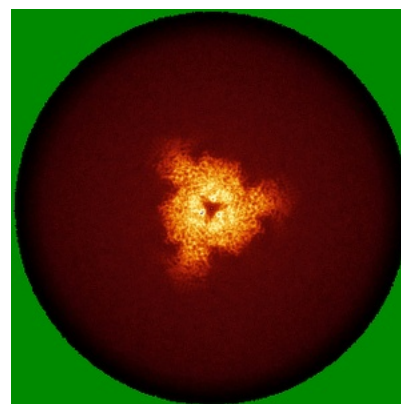
6.4.1 Primary map



X

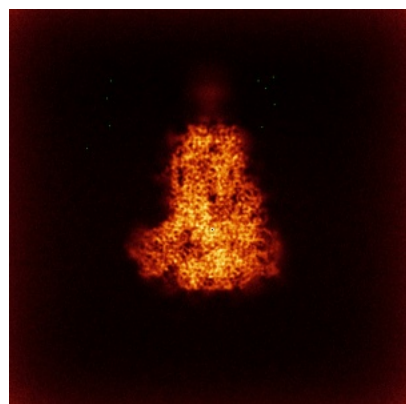


Y

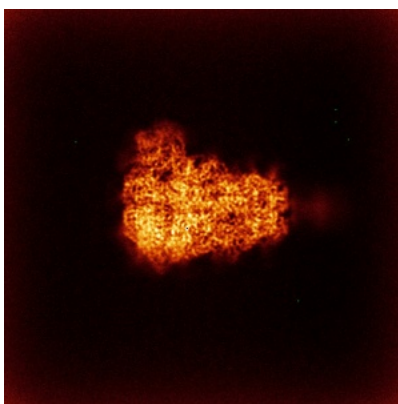


Z

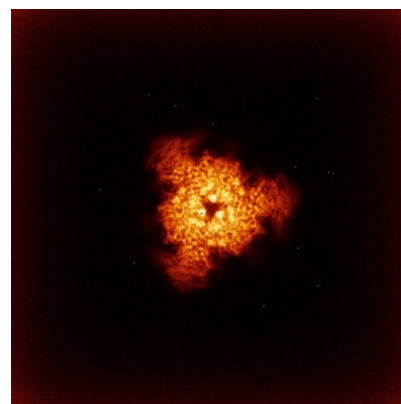
6.4.2 Raw map



X



Y

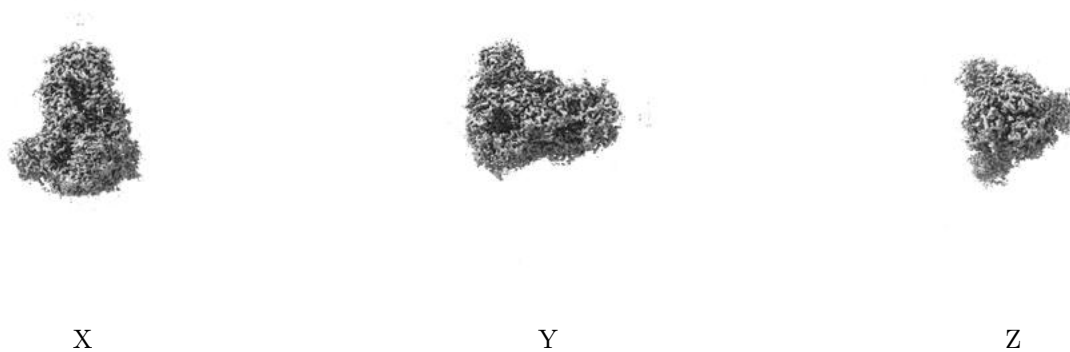


Z

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.

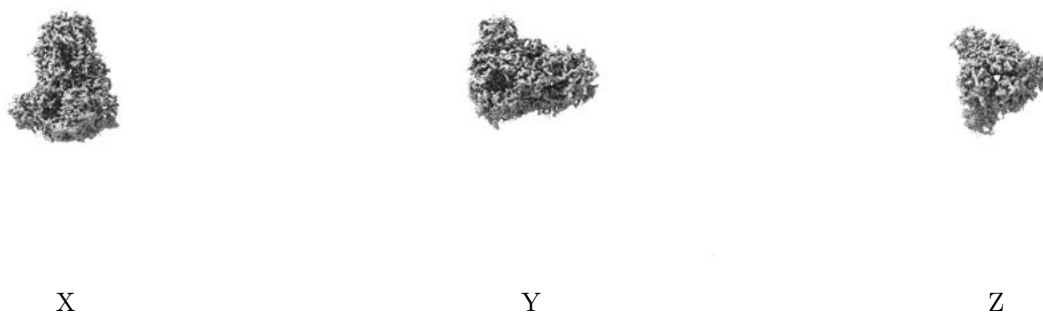
6.5 Orthogonal surface views [i](#)

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.

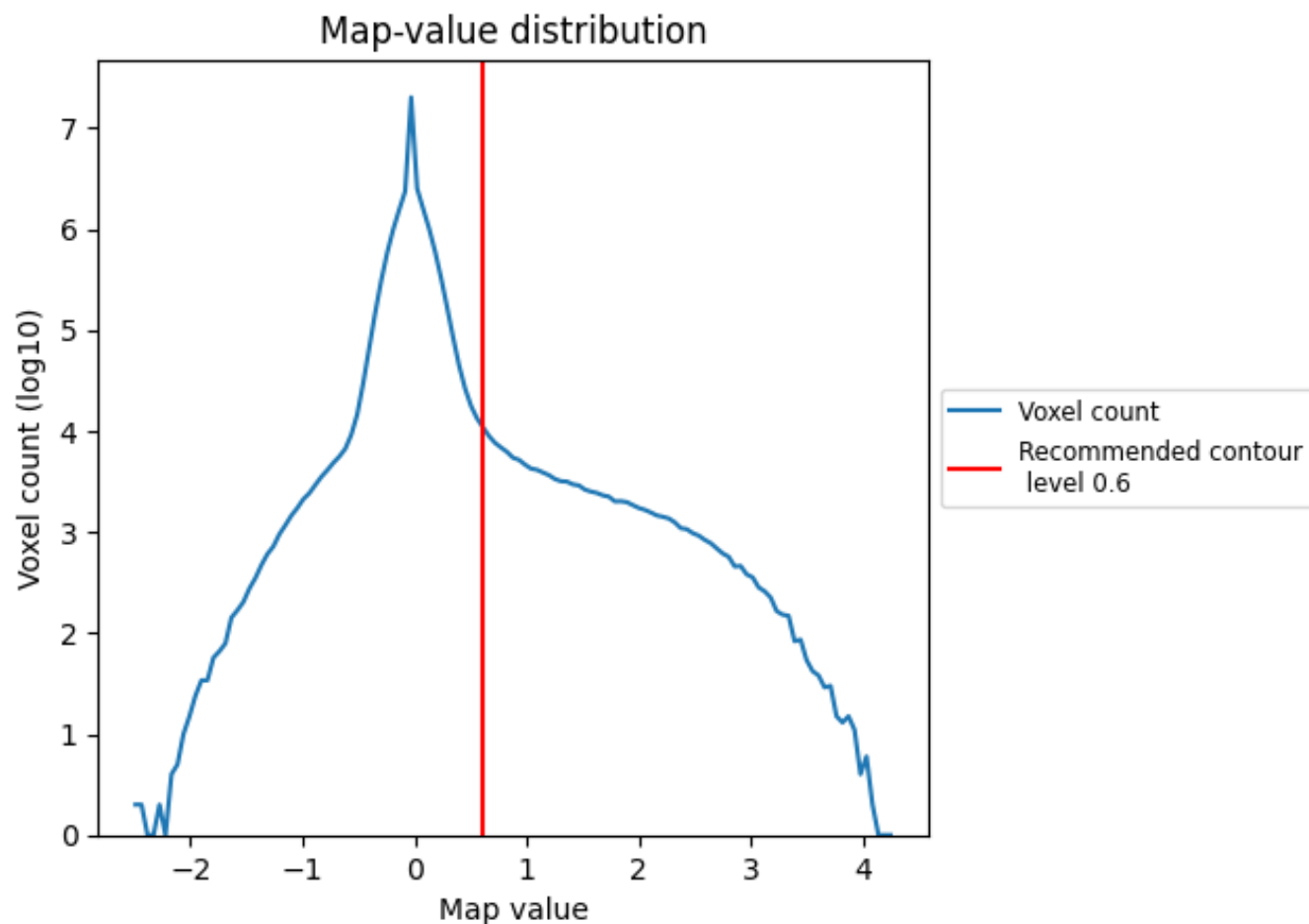
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

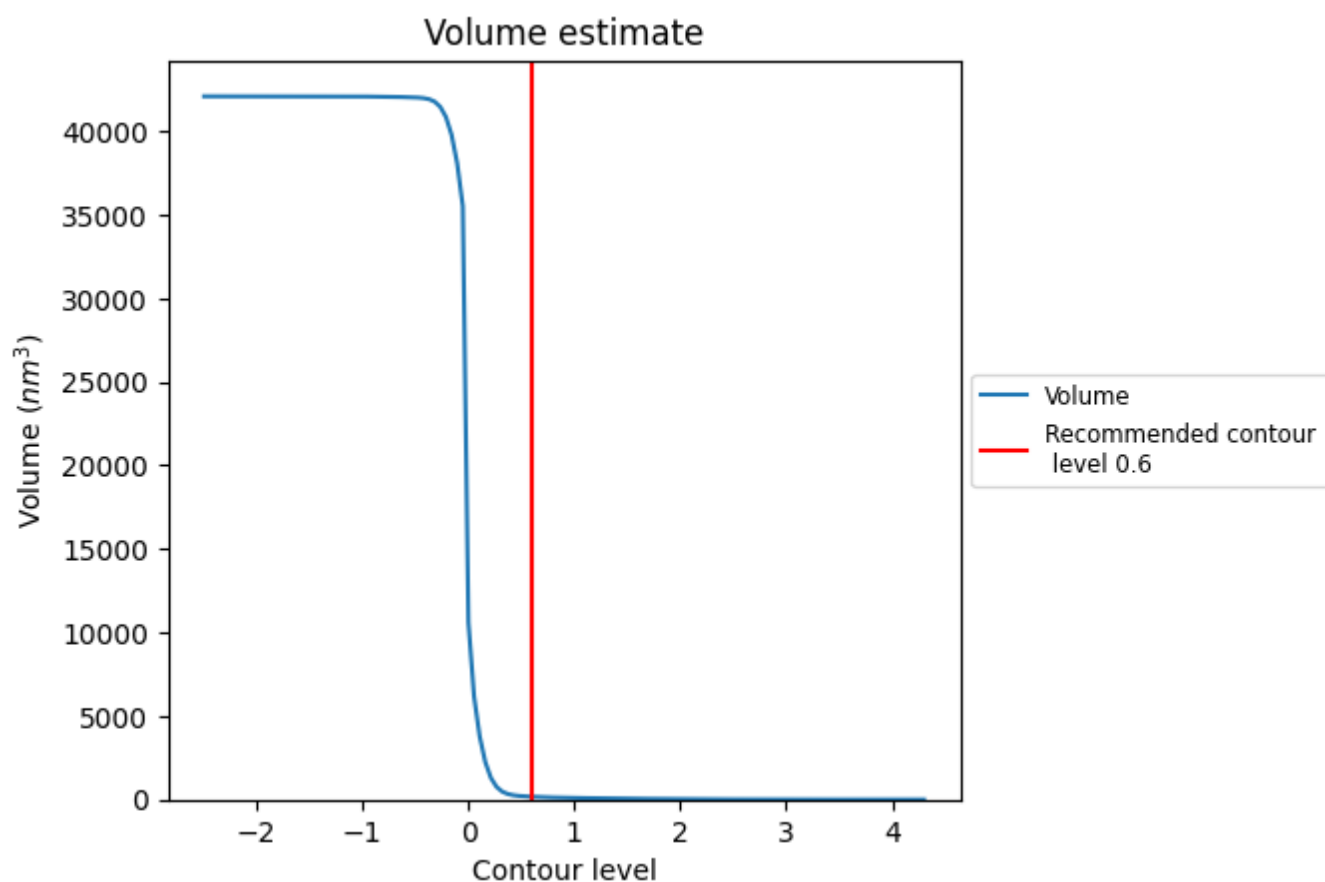
This section contains the results of statistical analysis of the map.

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.

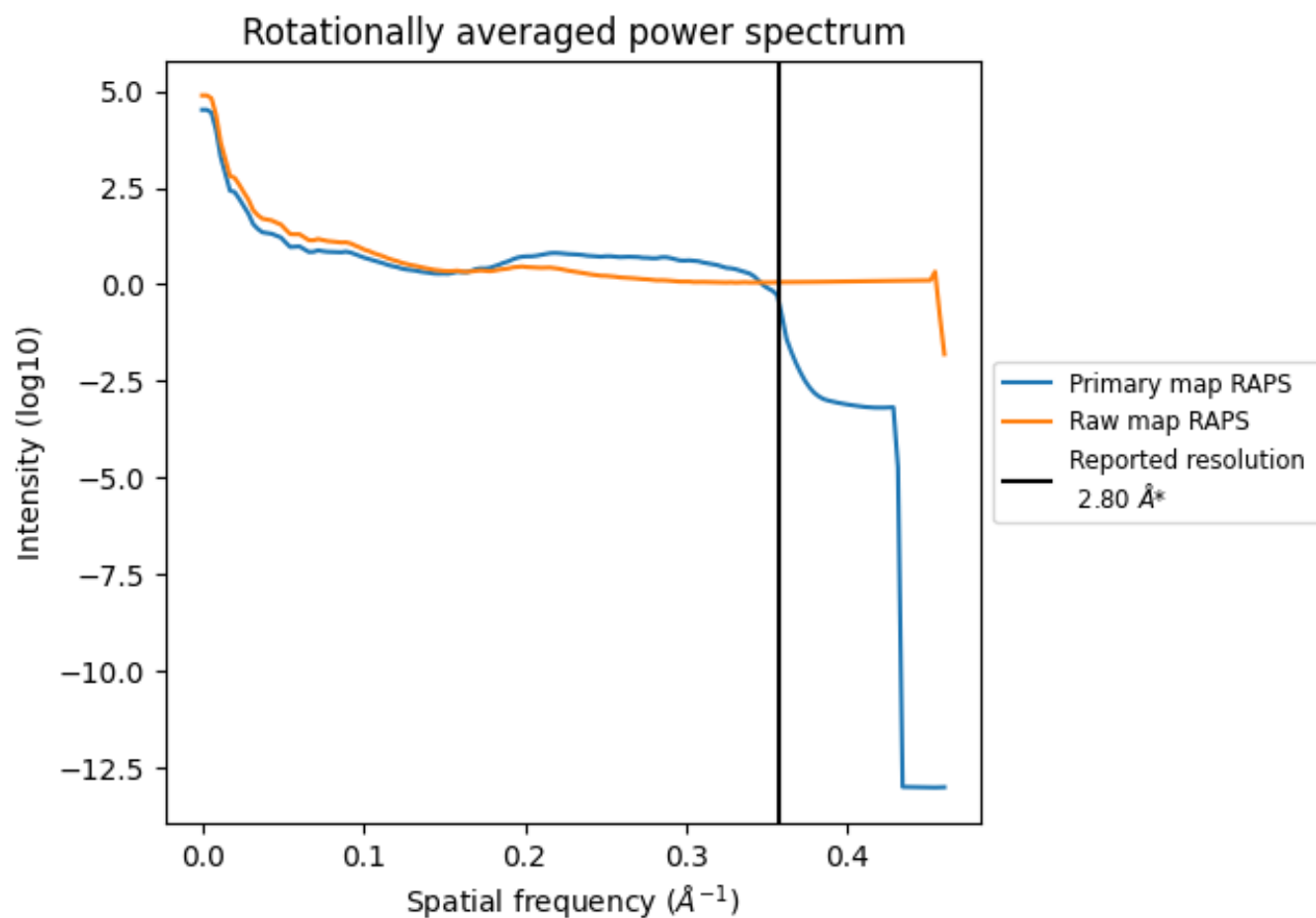
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm³; this corresponds to an approximate mass of 152 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 ⓘ

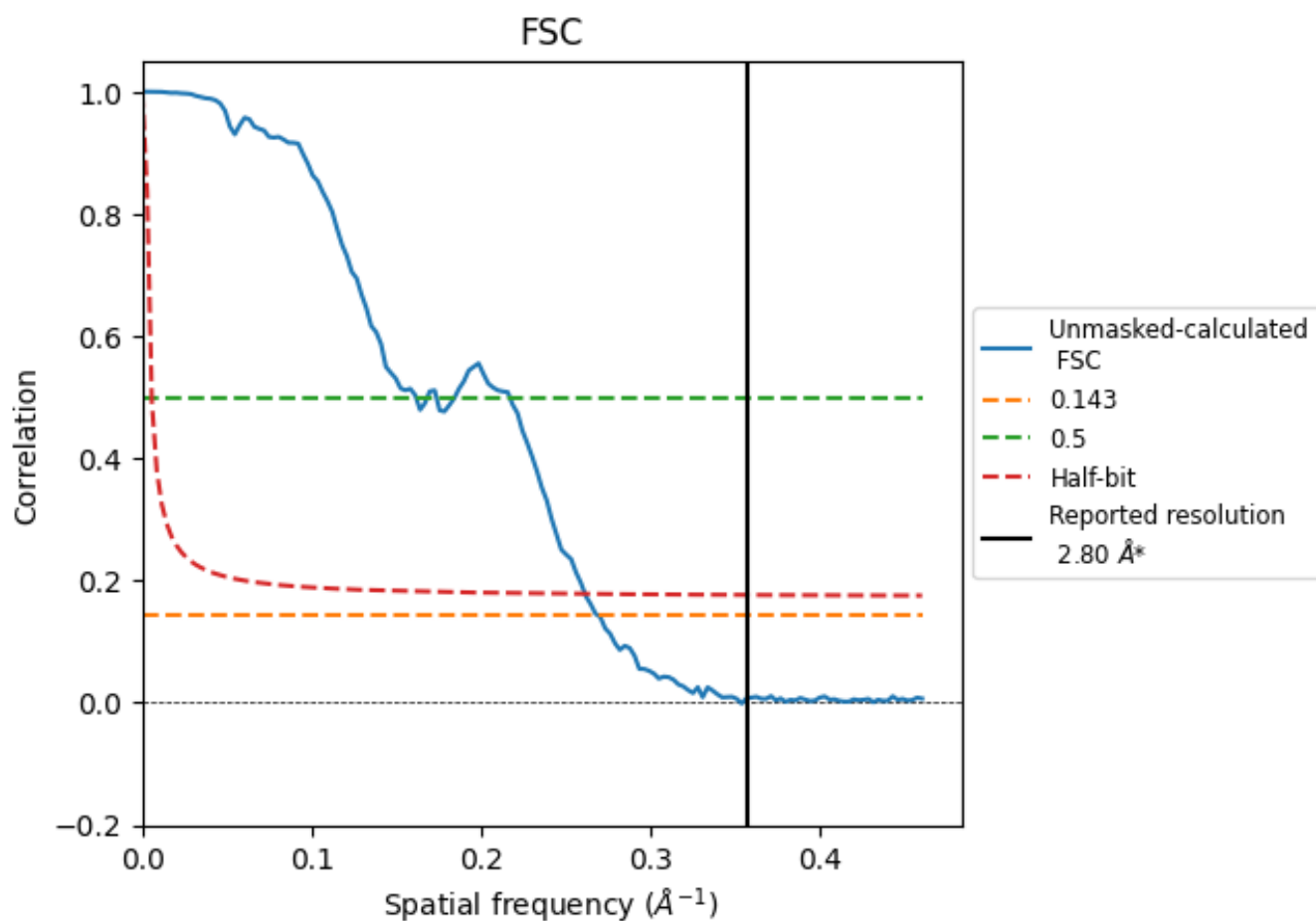


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

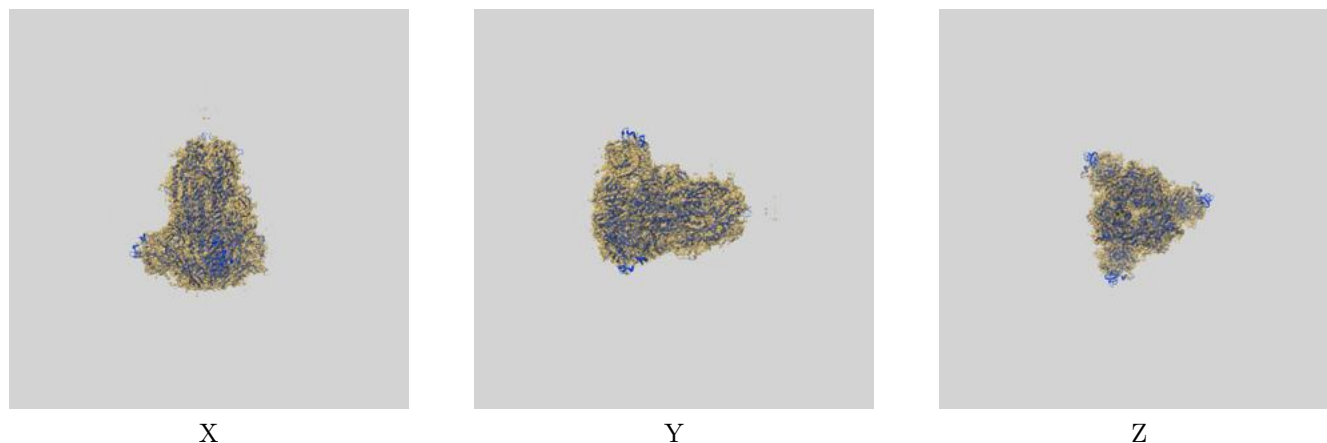
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.72	6.20	3.83

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

9 Map-model fit [i](#)

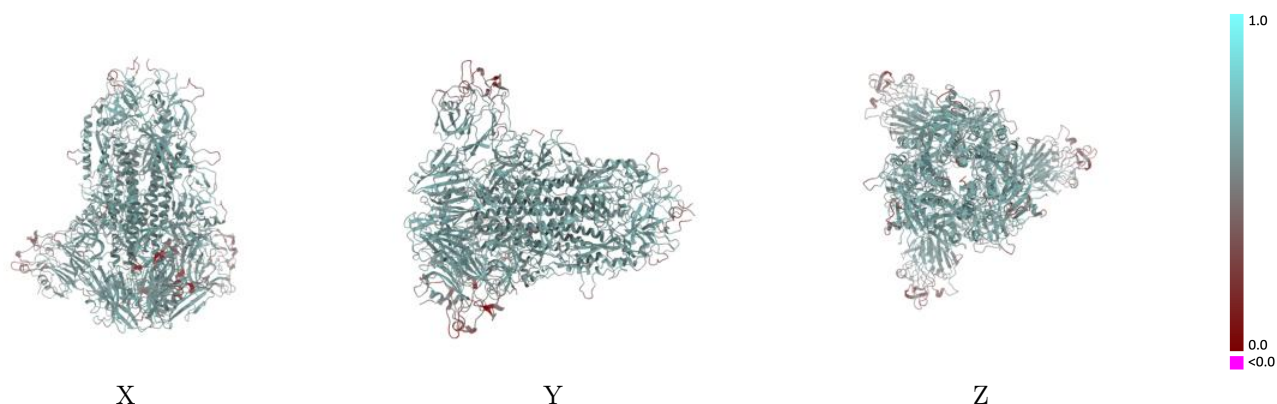
This section contains information regarding the fit between EMDB map EMD-62523 and PDB model 9KR9. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



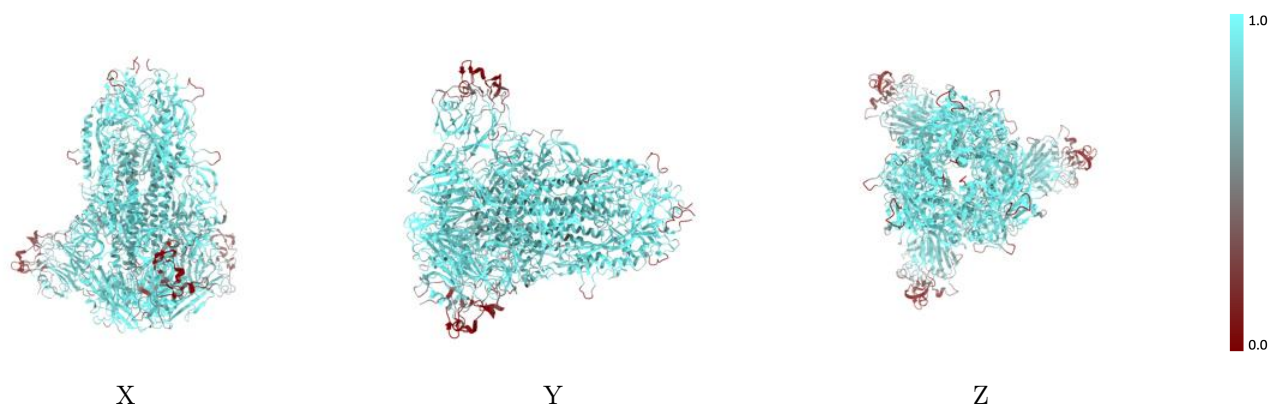
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



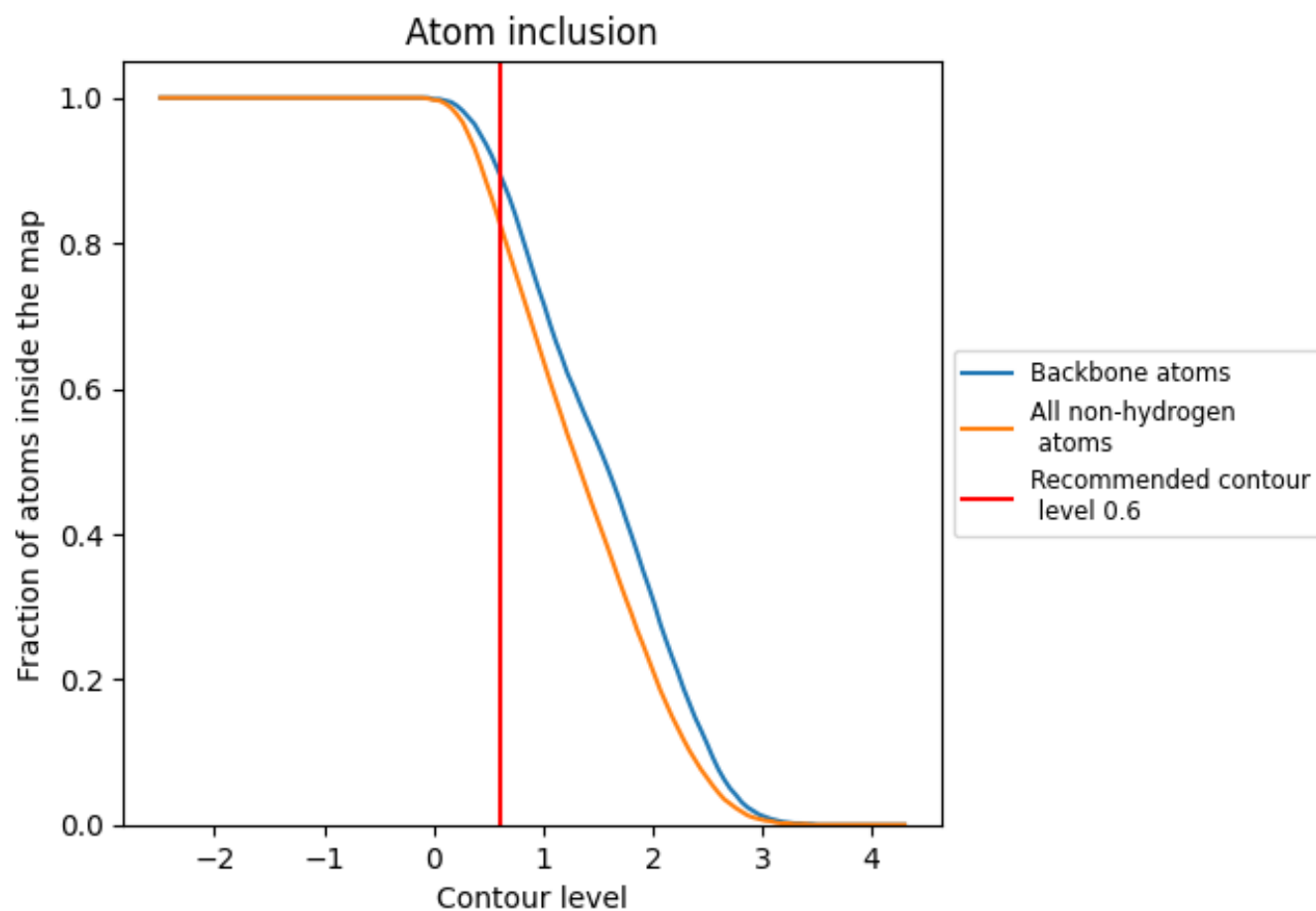
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 90% of all backbone atoms, 83% 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	 0.8300	 0.5740
A	 0.8380	 0.5760
B	 0.8370	 0.5770
C	 0.8380	 0.5770
D	 0.3210	 0.3540
E	 0.6430	 0.4860
F	 0.7140	 0.5350
G	 0.6910	 0.4770
H	 0.3930	 0.4450
I	 0.6790	 0.4790
J	 0.4290	 0.3660
K	 0.6070	 0.5120
L	 0.5710	 0.4790
M	 0.3210	 0.3650
N	 0.6430	 0.4810
O	 0.7140	 0.5330
P	 0.6670	 0.4830
Q	 0.3930	 0.4550
R	 0.6790	 0.4940
S	 0.4290	 0.3750
T	 0.5710	 0.5080
U	 0.5710	 0.4680
V	 0.3570	 0.3700
W	 0.6430	 0.4890
X	 0.7500	 0.5320
Y	 0.7140	 0.4850
Z	 0.4290	 0.4570
a	 0.6790	 0.4810
b	 0.4290	 0.3580
c	 0.6070	 0.5100
d	 0.5710	 0.4720

