



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 03:03 PM JST

PDB ID : 7CZZ
EMDB ID : EMD-30522
Title : S protein of SARS-CoV-2 in complex bound with P5A-2F11_3B
Authors : Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Zhou, Q.
Deposited on : 2020-09-09
Resolution : 3.20 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:

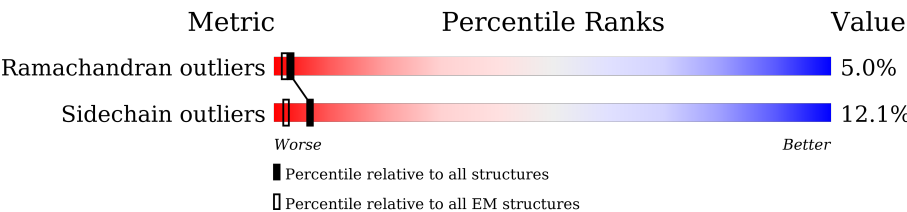
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1283	<div> <div>11%</div> <div>69%</div> <div>9%</div> <div>22%</div> </div>
1	B	1283	<div> <div>15%</div> <div>67%</div> <div>11%</div> <div>22%</div> </div>
1	C	1283	<div> <div>14%</div> <div>68%</div> <div>9%</div> <div>22%</div> </div>
2	H	452	<div> <div>49%</div> <div>42%</div> <div>7%</div> <div>50%</div> </div>
2	I	452	<div> <div>50%</div> <div>42%</div> <div>7%</div> <div>50%</div> </div>
2	J	452	<div> <div>50%</div> <div>42%</div> <div>7%</div> <div>50%</div> </div>
3	K	220	<div> <div>100%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>
3	M	220	<div> <div>100%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>
3	N	220	<div> <div>100%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	2	100%
4	E	2	100%
4	F	2	50%
4	G	2	50%
4	L	2	100%
4	O	2	50%
4	P	2	50%
4	Q	2	50%
4	R	2	100%
4	S	2	50%
4	T	2	50%
4	U	2	50%
4	V	2	50%
4	W	2	100%
4	X	2	50%
4	Y	2	100%
4	Z	2	50%
4	a	2	50%
4	b	2	50%
4	c	2	50%
4	d	2	100%
4	e	2	100%
5	f	3	33%
5	g	3	33%
5	h	3	33%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 34771 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	1006	Total	C	N	O	S	0	0
			7863	5019	1308	1500	36		
1	B	1007	Total	C	N	O	S	0	0
			7870	5023	1310	1501	36		
1	C	1004	Total	C	N	O	S	0	0
			7853	5014	1307	1496	36		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	ASP	-	expression tag	UNP P0DTC2
A	1277	TYR	-	expression tag	UNP P0DTC2
A	1278	LYS	-	expression tag	UNP P0DTC2
A	1279	ASP	-	expression tag	UNP P0DTC2
A	1280	ASP	-	expression tag	UNP P0DTC2
A	1281	ASP	-	expression tag	UNP P0DTC2
A	1282	ASP	-	expression tag	UNP P0DTC2
A	1283	LYS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	ASP	-	expression tag	UNP P0DTC2
B	1277	TYR	-	expression tag	UNP P0DTC2
B	1278	LYS	-	expression tag	UNP P0DTC2
B	1279	ASP	-	expression tag	UNP P0DTC2
B	1280	ASP	-	expression tag	UNP P0DTC2
B	1281	ASP	-	expression tag	UNP P0DTC2
B	1282	ASP	-	expression tag	UNP P0DTC2
B	1283	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	ASP	-	expression tag	UNP P0DTC2
C	1277	TYR	-	expression tag	UNP P0DTC2
C	1278	LYS	-	expression tag	UNP P0DTC2
C	1279	ASP	-	expression tag	UNP P0DTC2
C	1280	ASP	-	expression tag	UNP P0DTC2
C	1281	ASP	-	expression tag	UNP P0DTC2
C	1282	ASP	-	expression tag	UNP P0DTC2
C	1283	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Immunoglobulin heavy variable 1-8,Immunoglobulin heavy variable 1-8,chain H of P5A-2F11_3B,Epididymis luminal protein 214,Epididymis luminal protein 214.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	224	Total	C	N	O	S	0	0
			1670	1053	281	328	8		
2	I	224	Total	C	N	O	S	0	0
			1670	1053	281	328	8		
2	J	224	Total	C	N	O	S	0	0
			1670	1053	281	328	8		

- Molecule 3 is a protein called IG c168_light_IGKV4-1_IGKJ4,Immunoglobulin kappa constant.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	220	Total	C	N	O	S	0	0
			1685	1055	278	346	6		
3	M	220	Total	C	N	O	S	0	0
			1685	1055	278	346	6		
3	N	220	Total	C	N	O	S	0	0
			1685	1055	278	346	6		

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



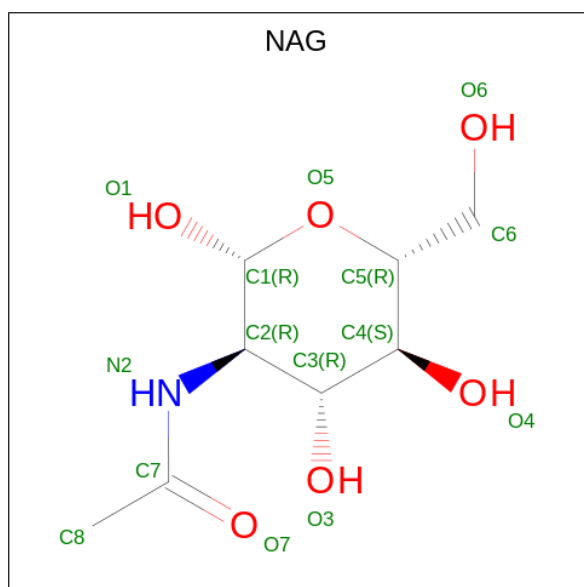
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total 28	C 16	N 2	O 10	0	0
4	E	2	Total 28	C 16	N 2	O 10	0	0
4	F	2	Total 28	C 16	N 2	O 10	0	0
4	G	2	Total 28	C 16	N 2	O 10	0	0
4	L	2	Total 28	C 16	N 2	O 10	0	0
4	O	2	Total 28	C 16	N 2	O 10	0	0
4	P	2	Total 28	C 16	N 2	O 10	0	0
4	Q	2	Total 28	C 16	N 2	O 10	0	0
4	R	2	Total 28	C 16	N 2	O 10	0	0
4	S	2	Total 28	C 16	N 2	O 10	0	0
4	T	2	Total 28	C 16	N 2	O 10	0	0
4	U	2	Total 28	C 16	N 2	O 10	0	0
4	V	2	Total 28	C 16	N 2	O 10	0	0
4	W	2	Total 28	C 16	N 2	O 10	0	0
4	X	2	Total 28	C 16	N 2	O 10	0	0
4	Y	2	Total 28	C 16	N 2	O 10	0	0
4	Z	2	Total 28	C 16	N 2	O 10	0	0
4	a	2	Total 28	C 16	N 2	O 10	0	0
4	b	2	Total 28	C 16	N 2	O 10	0	0
4	c	2	Total 28	C 16	N 2	O 10	0	0
4	d	2	Total 28	C 16	N 2	O 10	0	0
4	e	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 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
5	f	3	Total	C	N	O	0	0
			42	24	3	15		
5	g	3	Total	C	N	O	0	0
			42	24	3	15		
5	h	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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

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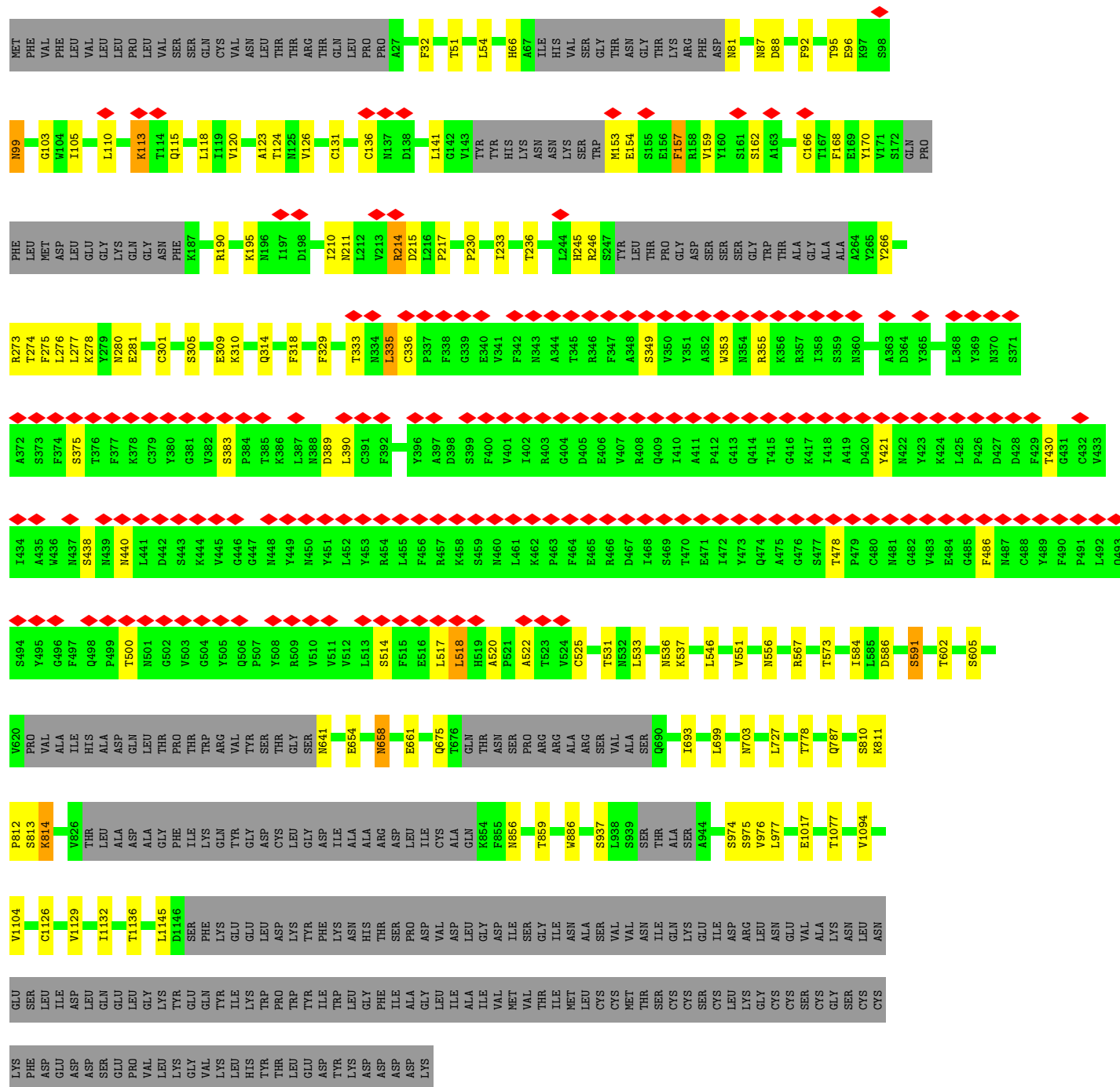
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	C	1	14	8	1	5	0



VAL	THR	PHE	ILE	PHE	MET	PHE	ASP	VAL	LEU	CYS	CYS	MET	THR	THR	CYS	CYS	SER	SER	CYS	CYS	LEU	LYS	GLY	ASN	VAL	LEU	LYS	GLY	VAL	LYS	LEU	HIS	THR	THR	LEU	GLU	ASP	ASP	LYS	ASP	ASP	ASP	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 1: Spike glycoprotein



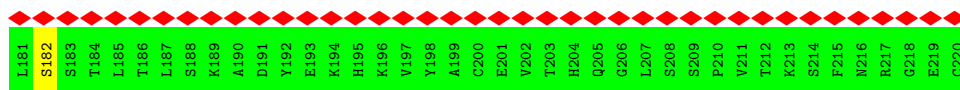
• Molecule 2: Immunoglobulin heavy variable 1-8,Immunoglobulin heavy variable 1-8,chain H of P5A-2F11_3B,Epididymis luminal protein 214,Epididymis luminal protein 214

Chain H:

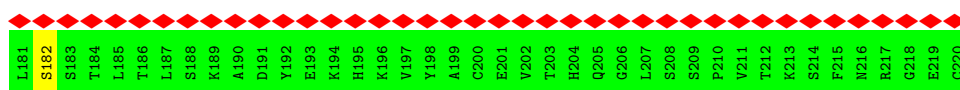
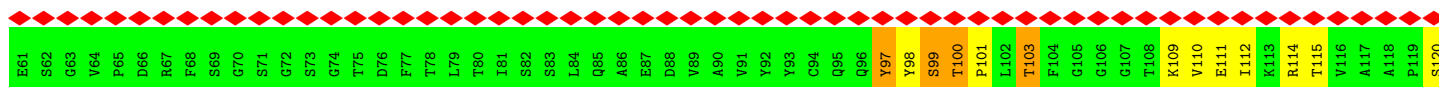
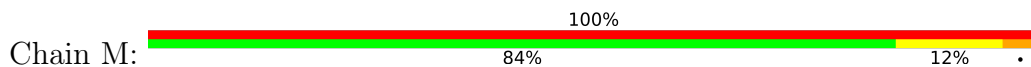
● Molecule 2: Immunoglobulin heavy variable 1-8,Immunoglobulin heavy variable 1-8,chain H of P5A-2F11_3B,Epididymis luminal protein 214,Epididymis luminal protein 214

Chain I:

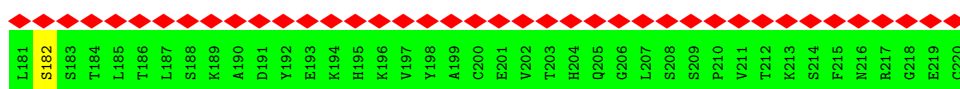
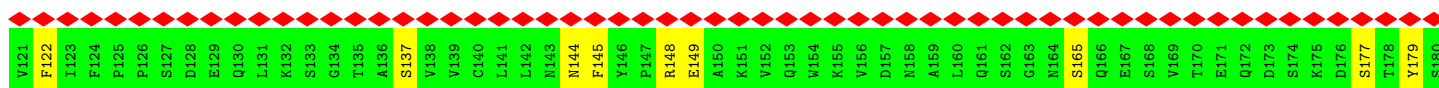
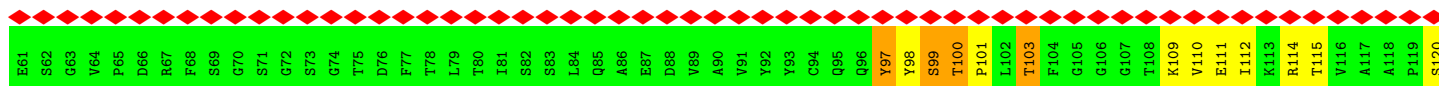
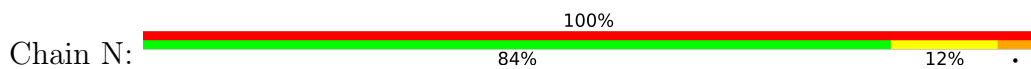
TYR
ASN
SER
THR
TYR
ARG



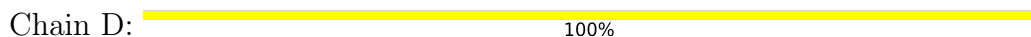
- Molecule 3: IG c168_light_IGKV4-1_IGKJ4,Immunoglobulin kappa constant



- Molecule 3: IG c168_light_IGKV4-1_IGKJ4,Immunoglobulin kappa constant



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



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



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



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



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



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





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

Chain d:  100%



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

Chain e:  100%



- Molecule 5: 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

Chain f:  100%
33% 67%



- Molecule 5: 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

Chain g:  100%
33% 67%



- Molecule 5: 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

Chain h:  100%
33% 67%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55704	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.175	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	0/8039	0.56	0/10936
1	B	0.71	0/8045	0.74	0/10942
1	C	0.71	0/8028	0.73	0/10919
2	H	0.36	0/1710	0.52	0/2331
2	I	0.36	0/1710	0.52	0/2331
2	J	0.36	0/1710	0.52	0/2331
3	K	0.46	0/1722	0.58	0/2343
3	M	0.46	0/1722	0.58	0/2343
3	N	0.46	0/1722	0.58	0/2343
All	All	0.61	0/34408	0.65	0/46819

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	988/1283 (77%)	870 (88%)	103 (10%)	15 (2%)	8	38
1	B	989/1283 (77%)	837 (85%)	111 (11%)	41 (4%)	2	17
1	C	986/1283 (77%)	850 (86%)	96 (10%)	40 (4%)	2	17
2	H	222/452 (49%)	175 (79%)	31 (14%)	16 (7%)	1	6
2	I	222/452 (49%)	175 (79%)	31 (14%)	16 (7%)	1	6
2	J	222/452 (49%)	175 (79%)	31 (14%)	16 (7%)	1	6
3	K	218/220 (99%)	162 (74%)	33 (15%)	23 (11%)	0	2
3	M	218/220 (99%)	162 (74%)	33 (15%)	23 (11%)	0	2
3	N	218/220 (99%)	162 (74%)	33 (15%)	23 (11%)	0	2
All	All	4283/5865 (73%)	3568 (83%)	502 (12%)	213 (5%)	3	13

All (213) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	LEU
1	A	518	LEU
1	A	983	ARG
1	B	97	LYS
1	B	133	PHE
1	B	159	VAL
1	B	163	ALA
1	B	239	GLN
1	B	285	ILE
1	B	325	SER
1	B	335	LEU
1	B	518	LEU
1	B	536	ASN
1	C	96	GLU
1	C	99	ASN
1	C	113	LYS
1	C	154	GLU
1	C	162	SER
1	C	233	ILE
1	C	274	THR
1	C	280	ASN
1	C	518	LEU
1	C	814	LYS

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Mol	Chain	Res	Type
2	H	55	SER
2	H	103	VAL
3	K	12	ALA
3	K	35	ASN
3	K	37	ASN
3	K	38	TYR
3	K	99	SER
3	K	100	THR
3	K	112	ILE
3	K	144	ASN
2	I	55	SER
2	I	103	VAL
3	M	12	ALA
3	M	35	ASN
3	M	37	ASN
3	M	38	TYR
3	M	99	SER
3	M	100	THR
3	M	112	ILE
3	M	144	ASN
2	J	55	SER
2	J	103	VAL
3	N	12	ALA
3	N	35	ASN
3	N	37	ASN
3	N	38	TYR
3	N	99	SER
3	N	100	THR
3	N	112	ILE
3	N	144	ASN
1	A	331	ASN
1	A	562	PHE
1	B	45	SER
1	B	89	GLY
1	B	161	SER
1	B	237	ARG
1	B	274	THR
1	B	280	ASN
1	B	532	ASN
1	B	557	LYS
1	B	562	PHE
1	C	103	GLY

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Mol	Chain	Res	Type
1	C	123	ALA
1	C	168	PHE
1	C	210	ILE
1	C	591	SER
1	C	810	SER
2	H	76	ILE
2	H	104	PRO
3	K	31	TYR
3	K	34	ASN
3	K	39	LEU
3	K	97	TYR
3	K	98	TYR
2	I	76	ILE
2	I	104	PRO
3	M	31	TYR
3	M	34	ASN
3	M	39	LEU
3	M	97	TYR
3	M	98	TYR
2	J	76	ILE
2	J	104	PRO
3	N	31	TYR
3	N	34	ASN
3	N	39	LEU
3	N	97	TYR
3	N	98	TYR
1	A	327	VAL
1	A	522	ALA
1	A	536	ASN
1	B	168	PHE
1	B	215	ASP
1	B	238	PHE
1	B	522	ALA
1	C	87	ASN
1	C	157	PHE
1	C	214	ARG
1	C	522	ALA
1	C	658	ASN
2	H	30	THR
2	H	31	SER
2	H	77	SER
2	H	121	SER

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Mol	Chain	Res	Type
3	K	17	GLU
3	K	103	THR
3	K	114	ARG
3	K	145	PHE
3	K	149	GLU
2	I	30	THR
2	I	31	SER
2	I	77	SER
2	I	121	SER
3	M	17	GLU
3	M	103	THR
3	M	114	ARG
3	M	145	PHE
2	J	30	THR
2	J	31	SER
2	J	77	SER
2	J	121	SER
3	N	17	GLU
3	N	103	THR
3	N	114	ARG
3	N	145	PHE
1	A	349	SER
1	A	520	ALA
1	A	982	SER
1	B	99	ASN
1	B	123	ALA
1	B	157	PHE
1	B	160	TYR
1	B	336	CYS
1	B	349	SER
1	B	520	ALA
1	B	529	LYS
1	B	560	LEU
1	C	32	PHE
1	C	211	ASN
1	C	349	SER
1	C	520	ALA
1	C	813	SER
2	H	29	PHE
2	H	124	SER
3	K	30	LEU
3	K	101	PRO

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Mol	Chain	Res	Type
3	K	115	THR
2	I	29	PHE
2	I	124	SER
3	M	30	LEU
3	M	101	PRO
3	M	115	THR
3	M	149	GLU
2	J	29	PHE
2	J	124	SER
3	N	30	LEU
3	N	101	PRO
3	N	115	THR
3	N	149	GLU
1	A	336	CYS
1	A	337	PRO
1	B	110	LEU
1	B	126	VAL
1	B	580	GLN
1	C	124	THR
1	C	126	VAL
1	C	159	VAL
1	C	217	PRO
1	C	281	GLU
1	C	335	LEU
1	C	336	CYS
1	C	531	THR
1	C	605	SER
1	C	661	GLU
1	C	812	PRO
2	H	47	TRP
2	H	56	GLY
2	H	111	PRO
3	K	109	LYS
2	I	47	TRP
2	I	56	GLY
2	I	111	PRO
3	M	109	LYS
2	J	47	TRP
2	J	56	GLY
2	J	111	PRO
3	N	109	LYS
1	A	560	LEU

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Mol	Chain	Res	Type
1	B	124	THR
1	B	582	LEU
1	C	230	PRO
1	C	329	PHE
1	C	811	LYS
2	H	53	PRO
2	H	110	ASP
2	I	53	PRO
2	I	110	ASP
2	J	53	PRO
2	J	110	ASP
3	K	110	VAL
3	M	110	VAL
3	N	110	VAL
1	A	579	PRO
1	B	39	PRO
1	B	142	GLY
1	B	103	GLY
2	H	113	GLY
2	I	113	GLY
2	J	113	GLY
1	B	337	PRO

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	881/1122 (78%)	774 (88%)	107 (12%)	4	19
1	B	881/1122 (78%)	763 (87%)	118 (13%)	3	15
1	C	879/1122 (78%)	780 (89%)	99 (11%)	4	22
2	H	188/399 (47%)	164 (87%)	24 (13%)	3	17
2	I	188/399 (47%)	164 (87%)	24 (13%)	3	17
2	J	188/399 (47%)	164 (87%)	24 (13%)	3	17
3	K	191/194 (98%)	170 (89%)	21 (11%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	191/194 (98%)	170 (89%)	21 (11%)	5	23
3	N	191/194 (98%)	170 (89%)	21 (11%)	5	23
All	All	3778/5145 (73%)	3319 (88%)	459 (12%)	6	19

All (459) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	A	97	LYS
1	A	109	THR
1	A	116	SER
1	A	118	LEU
1	A	122	ASN
1	A	137	ASN
1	A	141	LEU
1	A	143	VAL
1	A	158	ARG
1	A	164	ASN
1	A	169	GLU
1	A	195	LYS
1	A	205	SER
1	A	208	THR
1	A	221	SER
1	A	282	ASN
1	A	296	LEU
1	A	301	CYS
1	A	308	VAL
1	A	314	GLN
1	A	315	THR
1	A	318	PHE
1	A	324	GLU
1	A	325	SER
1	A	328	ARG
1	A	333	THR
1	A	335	LEU
1	A	353	TRP
1	A	355	ARG
1	A	375	SER
1	A	383	SER
1	A	389	ASP
1	A	390	LEU

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Mol	Chain	Res	Type
1	A	421	TYR
1	A	430	THR
1	A	438	SER
1	A	440	ASN
1	A	478	THR
1	A	486	PHE
1	A	500	THR
1	A	514	SER
1	A	517	LEU
1	A	518	LEU
1	A	525	CYS
1	A	528	LYS
1	A	529	LYS
1	A	530	SER
1	A	532	ASN
1	A	533	LEU
1	A	535	LYS
1	A	536	ASN
1	A	537	LYS
1	A	540	ASN
1	A	546	LEU
1	A	553	THR
1	A	556	ASN
1	A	558	LYS
1	A	576	VAL
1	A	578	ASP
1	A	580	GLN
1	A	583	GLU
1	A	588	THR
1	A	599	THR
1	A	602	THR
1	A	646	ARG
1	A	673	SER
1	A	698	SER
1	A	703	ASN
1	A	722	VAL
1	A	727	LEU
1	A	729	VAL
1	A	738	CYS
1	A	746	SER
1	A	773	GLU
1	A	785	VAL

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Mol	Chain	Res	Type
1	A	787	GLN
1	A	791	THR
1	A	826	VAL
1	A	868	GLU
1	A	878	LEU
1	A	883	THR
1	A	902	MET
1	A	916	LEU
1	A	929	SER
1	A	937	SER
1	A	939	SER
1	A	951	VAL
1	A	967	SER
1	A	983	ARG
1	A	985	ASP
1	A	988	GLU
1	A	994	ASP
1	A	1005	GLN
1	A	1074	ASN
1	A	1076	THR
1	A	1077	THR
1	A	1092	GLU
1	A	1094	VAL
1	A	1100	THR
1	A	1104	VAL
1	A	1123	SER
1	A	1125	ASN
1	A	1132	ILE
1	A	1141	LEU
1	A	1142	GLN
1	A	1144	GLU
1	B	33	THR
1	B	34	ARG
1	B	38	TYR
1	B	54	LEU
1	B	60	SER
1	B	62	VAL
1	B	83	VAL
1	B	92	PHE
1	B	97	LYS
1	B	101	ILE
1	B	105	ILE

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Mol	Chain	Res	Type
1	B	106	PHE
1	B	108	THR
1	B	114	THR
1	B	118	LEU
1	B	127	VAL
1	B	132	GLU
1	B	137	ASN
1	B	140	PHE
1	B	141	LEU
1	B	153	MET
1	B	157	PHE
1	B	158	ARG
1	B	160	TYR
1	B	161	SER
1	B	167	THR
1	B	190	ARG
1	B	195	LYS
1	B	196	ASN
1	B	210	ILE
1	B	212	LEU
1	B	214	ARG
1	B	217	PRO
1	B	223	LEU
1	B	229	LEU
1	B	238	PHE
1	B	246	ARG
1	B	266	TYR
1	B	270	LEU
1	B	273	ARG
1	B	276	LEU
1	B	282	ASN
1	B	287	ASP
1	B	298	GLU
1	B	307	THR
1	B	319	ARG
1	B	335	LEU
1	B	353	TRP
1	B	355	ARG
1	B	375	SER
1	B	383	SER
1	B	389	ASP
1	B	390	LEU

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Mol	Chain	Res	Type
1	B	421	TYR
1	B	430	THR
1	B	438	SER
1	B	440	ASN
1	B	478	THR
1	B	486	PHE
1	B	500	THR
1	B	514	SER
1	B	517	LEU
1	B	518	LEU
1	B	525	CYS
1	B	528	LYS
1	B	529	LYS
1	B	535	LYS
1	B	540	ASN
1	B	546	LEU
1	B	555	SER
1	B	556	ASN
1	B	557	LYS
1	B	558	LYS
1	B	565	PHE
1	B	580	GLN
1	B	581	THR
1	B	582	LEU
1	B	583	GLU
1	B	588	THR
1	B	591	SER
1	B	606	ASN
1	B	607	GLN
1	B	614	ASP
1	B	615	VAL
1	B	617	CYS
1	B	640	SER
1	B	649	CYS
1	B	676	THR
1	B	704	SER
1	B	710	ASN
1	B	746	SER
1	B	779	GLN
1	B	786	LYS
1	B	787	GLN
1	B	791	THR

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Mol	Chain	Res	Type
1	B	808	ASP
1	B	854	LYS
1	B	855	PHE
1	B	856	ASN
1	B	868	GLU
1	B	878	LEU
1	B	912	THR
1	B	916	LEU
1	B	935	GLN
1	B	964	LYS
1	B	968	SER
1	B	969	ASN
1	B	974	SER
1	B	976	VAL
1	B	1030	SER
1	B	1037	SER
1	B	1045	LYS
1	B	1074	ASN
1	B	1094	VAL
1	B	1104	VAL
1	B	1114	ILE
1	B	1126	CYS
1	B	1141	LEU
1	C	51	THR
1	C	54	LEU
1	C	66	HIS
1	C	81	ASN
1	C	88	ASP
1	C	92	PHE
1	C	95	THR
1	C	99	ASN
1	C	105	ILE
1	C	110	LEU
1	C	113	LYS
1	C	115	GLN
1	C	118	LEU
1	C	120	VAL
1	C	131	CYS
1	C	136	CYS
1	C	141	LEU
1	C	153	MET
1	C	157	PHE

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Mol	Chain	Res	Type
1	C	166	CYS
1	C	170	TYR
1	C	190	ARG
1	C	195	LYS
1	C	214	ARG
1	C	215	ASP
1	C	236	THR
1	C	245	HIS
1	C	246	ARG
1	C	266	TYR
1	C	273	ARG
1	C	275	PHE
1	C	276	LEU
1	C	277	LEU
1	C	278	LYS
1	C	301	CYS
1	C	305	SER
1	C	309	GLU
1	C	310	LYS
1	C	314	GLN
1	C	318	PHE
1	C	333	THR
1	C	335	LEU
1	C	353	TRP
1	C	355	ARG
1	C	375	SER
1	C	383	SER
1	C	389	ASP
1	C	390	LEU
1	C	421	TYR
1	C	430	THR
1	C	438	SER
1	C	440	ASN
1	C	478	THR
1	C	486	PHE
1	C	500	THR
1	C	514	SER
1	C	517	LEU
1	C	518	LEU
1	C	525	CYS
1	C	533	LEU
1	C	536	ASN

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Mol	Chain	Res	Type
1	C	537	LYS
1	C	546	LEU
1	C	551	VAL
1	C	556	ASN
1	C	567	ARG
1	C	573	THR
1	C	584	ILE
1	C	586	ASP
1	C	591	SER
1	C	602	THR
1	C	641	ASN
1	C	654	GLU
1	C	658	ASN
1	C	675	GLN
1	C	693	ILE
1	C	699	LEU
1	C	703	ASN
1	C	727	LEU
1	C	778	THR
1	C	787	GLN
1	C	814	LYS
1	C	856	ASN
1	C	859	THR
1	C	886	TRP
1	C	937	SER
1	C	974	SER
1	C	975	SER
1	C	976	VAL
1	C	977	LEU
1	C	1017	GLU
1	C	1077	THR
1	C	1094	VAL
1	C	1104	VAL
1	C	1126	CYS
1	C	1129	VAL
1	C	1132	ILE
1	C	1136	THR
1	C	1145	LEU
2	H	30	THR
2	H	33	ASP
2	H	47	TRP
2	H	50	TRP

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Mol	Chain	Res	Type
2	H	51	MET
2	H	69	THR
2	H	76	ILE
2	H	78	THR
2	H	103	VAL
2	H	107	LYS
2	H	109	PHE
2	H	112	TRP
2	H	122	SER
2	H	129	SER
2	H	141	SER
2	H	147	LEU
2	H	151	VAL
2	H	169	THR
2	H	173	HIS
2	H	182	SER
2	H	188	SER
2	H	206	ASN
2	H	210	LYS
2	H	217	ASP
3	K	6	GLN
3	K	15	LEU
3	K	17	GLU
3	K	31	TYR
3	K	37	ASN
3	K	38	TYR
3	K	39	LEU
3	K	59	THR
3	K	97	TYR
3	K	99	SER
3	K	100	THR
3	K	103	THR
3	K	111	GLU
3	K	120	SER
3	K	122	PHE
3	K	137	SER
3	K	148	ARG
3	K	165	SER
3	K	177	SER
3	K	179	TYR
3	K	182	SER
2	I	30	THR

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Mol	Chain	Res	Type
2	I	33	ASP
2	I	47	TRP
2	I	50	TRP
2	I	51	MET
2	I	69	THR
2	I	76	ILE
2	I	78	THR
2	I	103	VAL
2	I	107	LYS
2	I	109	PHE
2	I	112	TRP
2	I	122	SER
2	I	129	SER
2	I	141	SER
2	I	147	LEU
2	I	151	VAL
2	I	169	THR
2	I	173	HIS
2	I	182	SER
2	I	188	SER
2	I	206	ASN
2	I	210	LYS
2	I	217	ASP
3	M	6	GLN
3	M	15	LEU
3	M	17	GLU
3	M	31	TYR
3	M	37	ASN
3	M	38	TYR
3	M	39	LEU
3	M	59	THR
3	M	97	TYR
3	M	99	SER
3	M	100	THR
3	M	103	THR
3	M	111	GLU
3	M	120	SER
3	M	122	PHE
3	M	137	SER
3	M	148	ARG
3	M	165	SER
3	M	177	SER

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Mol	Chain	Res	Type
3	M	179	TYR
3	M	182	SER
2	J	30	THR
2	J	33	ASP
2	J	47	TRP
2	J	50	TRP
2	J	51	MET
2	J	69	THR
2	J	76	ILE
2	J	78	THR
2	J	103	VAL
2	J	107	LYS
2	J	109	PHE
2	J	112	TRP
2	J	122	SER
2	J	129	SER
2	J	141	SER
2	J	147	LEU
2	J	151	VAL
2	J	169	THR
2	J	173	HIS
2	J	182	SER
2	J	188	SER
2	J	206	ASN
2	J	210	LYS
2	J	217	ASP
3	N	6	GLN
3	N	15	LEU
3	N	17	GLU
3	N	31	TYR
3	N	37	ASN
3	N	38	TYR
3	N	39	LEU
3	N	59	THR
3	N	97	TYR
3	N	99	SER
3	N	100	THR
3	N	103	THR
3	N	111	GLU
3	N	120	SER
3	N	122	PHE
3	N	137	SER

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Mol	Chain	Res	Type
3	N	148	ARG
3	N	165	SER
3	N	177	SER
3	N	179	TYR
3	N	182	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	137	ASN
1	A	188	ASN
1	A	239	GLN
1	A	354	ASN
1	A	360	ASN
1	A	394	ASN
1	A	422	ASN
1	A	440	ASN
1	A	481	ASN
1	A	493	GLN
1	A	498	GLN
1	A	532	ASN
1	A	540	ASN
1	A	556	ASN
1	A	564	GLN
1	A	580	GLN
1	A	644	GLN
1	A	658	ASN
1	A	690	GLN
1	A	703	ASN
1	A	762	GLN
1	A	787	GLN
1	A	856	ASN
1	A	901	GLN
1	A	914	ASN
1	A	919	ASN
1	A	926	GLN
1	A	955	ASN
1	A	969	ASN
1	A	992	GLN
1	A	1125	ASN
1	A	1142	GLN

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Mol	Chain	Res	Type
1	B	81	ASN
1	B	115	GLN
1	B	125	ASN
1	B	137	ASN
1	B	164	ASN
1	B	239	GLN
1	B	245	HIS
1	B	354	ASN
1	B	360	ASN
1	B	394	ASN
1	B	422	ASN
1	B	440	ASN
1	B	481	ASN
1	B	493	GLN
1	B	498	GLN
1	B	540	ASN
1	B	556	ASN
1	B	564	GLN
1	B	580	GLN
1	B	606	ASN
1	B	607	GLN
1	B	710	ASN
1	B	804	GLN
1	B	901	GLN
1	B	914	ASN
1	B	919	ASN
1	B	920	GLN
1	B	926	GLN
1	B	992	GLN
1	B	1054	GLN
1	C	30	ASN
1	C	66	HIS
1	C	87	ASN
1	C	125	ASN
1	C	196	ASN
1	C	314	GLN
1	C	321	GLN
1	C	354	ASN
1	C	360	ASN
1	C	394	ASN
1	C	422	ASN
1	C	440	ASN

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Mol	Chain	Res	Type
1	C	481	ASN
1	C	493	GLN
1	C	498	GLN
1	C	536	ASN
1	C	556	ASN
1	C	641	ASN
1	C	655	HIS
1	C	675	GLN
1	C	703	ASN
1	C	784	GLN
1	C	804	GLN
1	C	901	GLN
1	C	907	ASN
1	C	914	ASN
1	C	926	GLN
1	C	935	GLN
1	C	969	ASN
1	C	992	GLN
1	C	1010	GLN
1	C	1071	GLN
1	C	1101	HIS
1	C	1106	GLN
2	H	6	GLN
3	K	43	GLN
3	K	96	GLN
2	I	6	GLN
3	M	43	GLN
3	M	96	GLN
2	J	6	GLN
3	N	6	GLN
3	N	43	GLN
3	N	96	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

53 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	$\# Z > 2$
4	NAG	D	1	4,1	14,14,15	0.41	0	17,19,21	1.17	1 (5%)
4	NAG	D	2	4	14,14,15	0.42	0	17,19,21	1.16	1 (5%)
4	NAG	E	1	4,1	14,14,15	0.54	0	17,19,21	0.57	0
4	NAG	E	2	4	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	F	1	4,1	14,14,15	0.36	0	17,19,21	0.63	1 (5%)
4	NAG	F	2	4	14,14,15	0.52	0	17,19,21	0.46	0
4	NAG	G	1	4,1	14,14,15	0.39	0	17,19,21	0.73	0
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	1.31	2 (11%)
4	NAG	L	1	4,1	14,14,15	0.70	1 (7%)	17,19,21	0.70	0
4	NAG	L	2	4	14,14,15	0.40	0	17,19,21	1.38	3 (17%)
4	NAG	O	1	4,1	14,14,15	0.70	1 (7%)	17,19,21	0.66	0
4	NAG	O	2	4	14,14,15	0.30	0	17,19,21	0.65	0
4	NAG	P	1	4,1	14,14,15	0.24	0	17,19,21	0.71	1 (5%)
4	NAG	P	2	4	14,14,15	0.15	0	17,19,21	0.44	0
4	NAG	Q	1	4,1	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
4	NAG	Q	2	4	14,14,15	0.31	0	17,19,21	0.61	0
4	NAG	R	1	4,1	14,14,15	0.56	0	17,19,21	0.57	0
4	NAG	R	2	4	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	S	1	4,1	14,14,15	0.33	0	17,19,21	0.41	0
4	NAG	S	2	4	14,14,15	0.38	0	17,19,21	0.36	0
4	NAG	T	1	4,1	14,14,15	0.34	0	17,19,21	1.10	1 (5%)
4	NAG	T	2	4	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	U	1	4,1	14,14,15	0.31	0	17,19,21	0.69	1 (5%)
4	NAG	U	2	4	14,14,15	0.21	0	17,19,21	0.39	0
4	NAG	V	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	V	2	4	14,14,15	0.30	0	17,19,21	0.67	0
4	NAG	W	1	4,1	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	W	2	4	14,14,15	0.28	0	17,19,21	0.38	0
4	NAG	X	1	4,1	14,14,15	0.40	0	17,19,21	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	X	2	4	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
4	NAG	Y	1	4,1	14,14,15	0.56	0	17,19,21	0.57	0
4	NAG	Y	2	4	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	Z	1	4,1	14,14,15	0.21	0	17,19,21	1.35	1 (5%)
4	NAG	Z	2	4	14,14,15	0.19	0	17,19,21	0.50	0
4	NAG	a	1	4,1	14,14,15	0.52	0	17,19,21	0.71	1 (5%)
4	NAG	a	2	4	14,14,15	0.41	0	17,19,21	0.46	0
4	NAG	b	1	4,1	14,14,15	0.34	0	17,19,21	0.42	0
4	NAG	b	2	4	14,14,15	0.23	0	17,19,21	0.72	0
4	NAG	c	1	4,1	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	c	2	4	14,14,15	0.55	0	17,19,21	1.31	1 (5%)
4	NAG	d	1	4,1	14,14,15	0.63	1 (7%)	17,19,21	0.45	0
4	NAG	d	2	4	14,14,15	0.30	0	17,19,21	1.34	2 (11%)
4	NAG	e	1	4,1	14,14,15	0.41	0	17,19,21	0.43	0
4	NAG	e	2	4	14,14,15	0.24	0	17,19,21	0.48	0
5	NAG	f	1	2,5	14,14,15	0.41	0	17,19,21	1.17	1 (5%)
5	NAG	f	2	5	14,14,15	0.31	0	17,19,21	0.99	1 (5%)
5	NAG	f	3	5	14,14,15	0.29	0	17,19,21	0.62	0
5	NAG	g	1	2,5	14,14,15	0.41	0	17,19,21	1.18	1 (5%)
5	NAG	g	2	5	14,14,15	0.30	0	17,19,21	0.99	1 (5%)
5	NAG	g	3	5	14,14,15	0.28	0	17,19,21	0.62	0
5	NAG	h	1	2,5	14,14,15	0.40	0	17,19,21	1.17	1 (5%)
5	NAG	h	2	5	14,14,15	0.30	0	17,19,21	0.99	1 (5%)
5	NAG	h	3	5	14,14,15	0.29	0	17,19,21	0.62	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
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	5/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	3/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	5/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	4/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	1/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	3/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	3/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	4/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	6/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	NAG	a	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	NAG	b	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	1/6/23/26	0/1/1/1
4	NAG	c	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	c	2	4	-	5/6/23/26	0/1/1/1
4	NAG	d	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	4/6/23/26	0/1/1/1
4	NAG	e	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	e	2	4	-	2/6/23/26	0/1/1/1
5	NAG	f	1	2,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	f	2	5	-	4/6/23/26	0/1/1/1
5	NAG	f	3	5	-	2/6/23/26	0/1/1/1
5	NAG	g	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	g	2	5	-	4/6/23/26	0/1/1/1
5	NAG	g	3	5	-	2/6/23/26	0/1/1/1
5	NAG	h	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	h	2	5	-	4/6/23/26	0/1/1/1
5	NAG	h	3	5	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1	NAG	O5-C1	-2.79	1.39	1.43
4	O	1	NAG	O5-C1	-2.55	1.39	1.43
4	L	1	NAG	O5-C1	-2.37	1.39	1.43
4	d	1	NAG	O5-C1	-2.12	1.40	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Z	1	NAG	C2-N2-C7	4.59	129.44	122.90
4	c	2	NAG	C2-N2-C7	4.35	129.10	122.90
4	d	2	NAG	C2-N2-C7	4.32	129.06	122.90
4	L	2	NAG	C2-N2-C7	4.29	129.01	122.90
4	G	2	NAG	C2-N2-C7	4.28	129.00	122.90
4	T	1	NAG	C1-O5-C5	3.23	116.56	112.19
4	L	2	NAG	C1-C2-N2	2.46	114.69	110.49
4	V	1	NAG	O4-C4-C3	-2.41	104.78	110.35
5	g	1	NAG	C8-C7-N2	2.37	120.12	116.10
5	f	1	NAG	C8-C7-N2	2.37	120.11	116.10
5	h	2	NAG	O5-C1-C2	-2.36	107.56	111.29
5	h	1	NAG	C8-C7-N2	2.36	120.09	116.10
5	g	2	NAG	O5-C1-C2	-2.36	107.57	111.29
4	D	1	NAG	C8-C7-N2	2.36	120.09	116.10
4	X	2	NAG	C8-C7-N2	2.35	120.08	116.10
5	f	2	NAG	O5-C1-C2	-2.34	107.59	111.29
4	Q	1	NAG	C8-C7-N2	2.32	120.02	116.10
4	D	2	NAG	C8-C7-N2	2.31	120.00	116.10
4	d	2	NAG	C1-C2-N2	2.29	114.39	110.49
4	X	1	NAG	C8-C7-N2	2.28	119.97	116.10
4	a	1	NAG	C1-O5-C5	2.26	115.25	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	1	NAG	C1-O5-C5	2.26	115.25	112.19
4	U	1	NAG	C1-O5-C5	2.25	115.25	112.19
4	G	2	NAG	C1-C2-N2	2.22	114.28	110.49
4	X	1	NAG	C2-N2-C7	-2.11	119.90	122.90
4	L	2	NAG	C1-O5-C5	2.09	115.03	112.19
4	F	1	NAG	C1-O5-C5	2.02	114.94	112.19
4	Q	1	NAG	C2-N2-C7	-2.01	120.04	122.90
4	X	2	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
5	f	2	NAG	C8-C7-N2-C2
5	f	2	NAG	O7-C7-N2-C2
5	g	2	NAG	C8-C7-N2-C2
5	g	2	NAG	O7-C7-N2-C2
5	h	2	NAG	C8-C7-N2-C2
5	h	2	NAG	O7-C7-N2-C2
4	Z	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	U	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	U	2	NAG	O7-C7-N2-C2
4	Z	1	NAG	C8-C7-N2-C2
4	Z	1	NAG	O7-C7-N2-C2
4	c	2	NAG	C8-C7-N2-C2
4	c	2	NAG	O7-C7-N2-C2
4	d	2	NAG	C8-C7-N2-C2
4	d	2	NAG	O7-C7-N2-C2
4	W	2	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	Q	2	NAG	C1-C2-N2-C7
5	f	3	NAG	C8-C7-N2-C2
5	g	3	NAG	C8-C7-N2-C2
5	h	3	NAG	C8-C7-N2-C2
4	O	2	NAG	O5-C5-C6-O6
5	f	2	NAG	C1-C2-N2-C7
5	g	2	NAG	C1-C2-N2-C7
5	h	2	NAG	C1-C2-N2-C7
4	d	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
5	f	3	NAG	O7-C7-N2-C2
5	g	3	NAG	O7-C7-N2-C2
5	h	3	NAG	O7-C7-N2-C2
4	E	2	NAG	C1-C2-N2-C7
4	R	2	NAG	C1-C2-N2-C7
4	Y	2	NAG	C1-C2-N2-C7
4	d	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	C3-C2-N2-C7
4	U	2	NAG	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6

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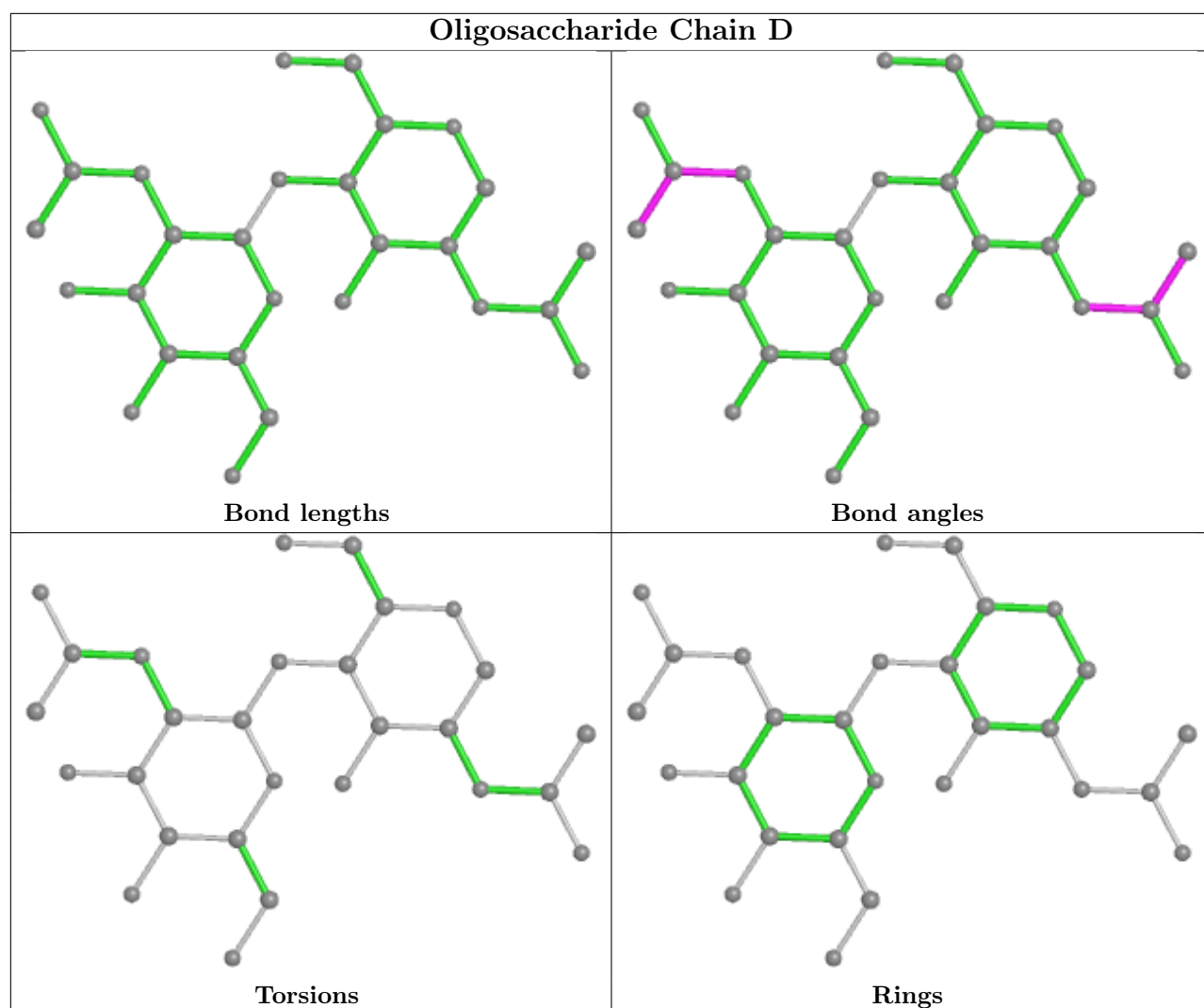
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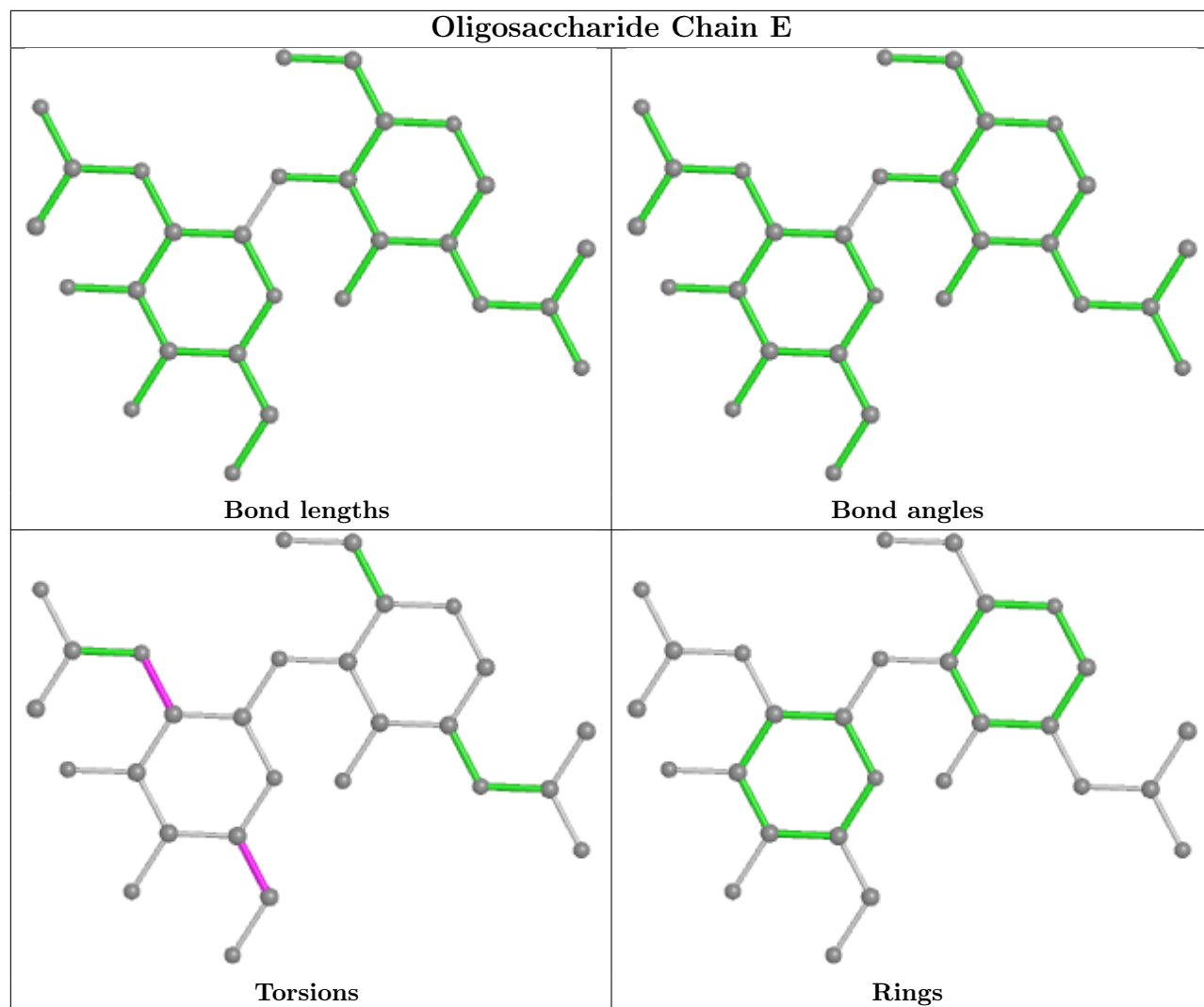
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	C4-C5-C6-O6
4	e	2	NAG	C4-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C3-C2-N2-C7
4	T	1	NAG	C3-C2-N2-C7
4	V	2	NAG	C3-C2-N2-C7
4	b	2	NAG	C3-C2-N2-C7
5	f	2	NAG	C3-C2-N2-C7
5	g	2	NAG	C3-C2-N2-C7
5	h	2	NAG	C3-C2-N2-C7
4	L	2	NAG	C4-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	C1-C2-N2-C7
4	E	2	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7
4	L	2	NAG	C3-C2-N2-C7
4	R	2	NAG	C3-C2-N2-C7
4	Y	2	NAG	C3-C2-N2-C7
4	Z	1	NAG	C3-C2-N2-C7
4	c	2	NAG	C3-C2-N2-C7
4	d	2	NAG	C3-C2-N2-C7

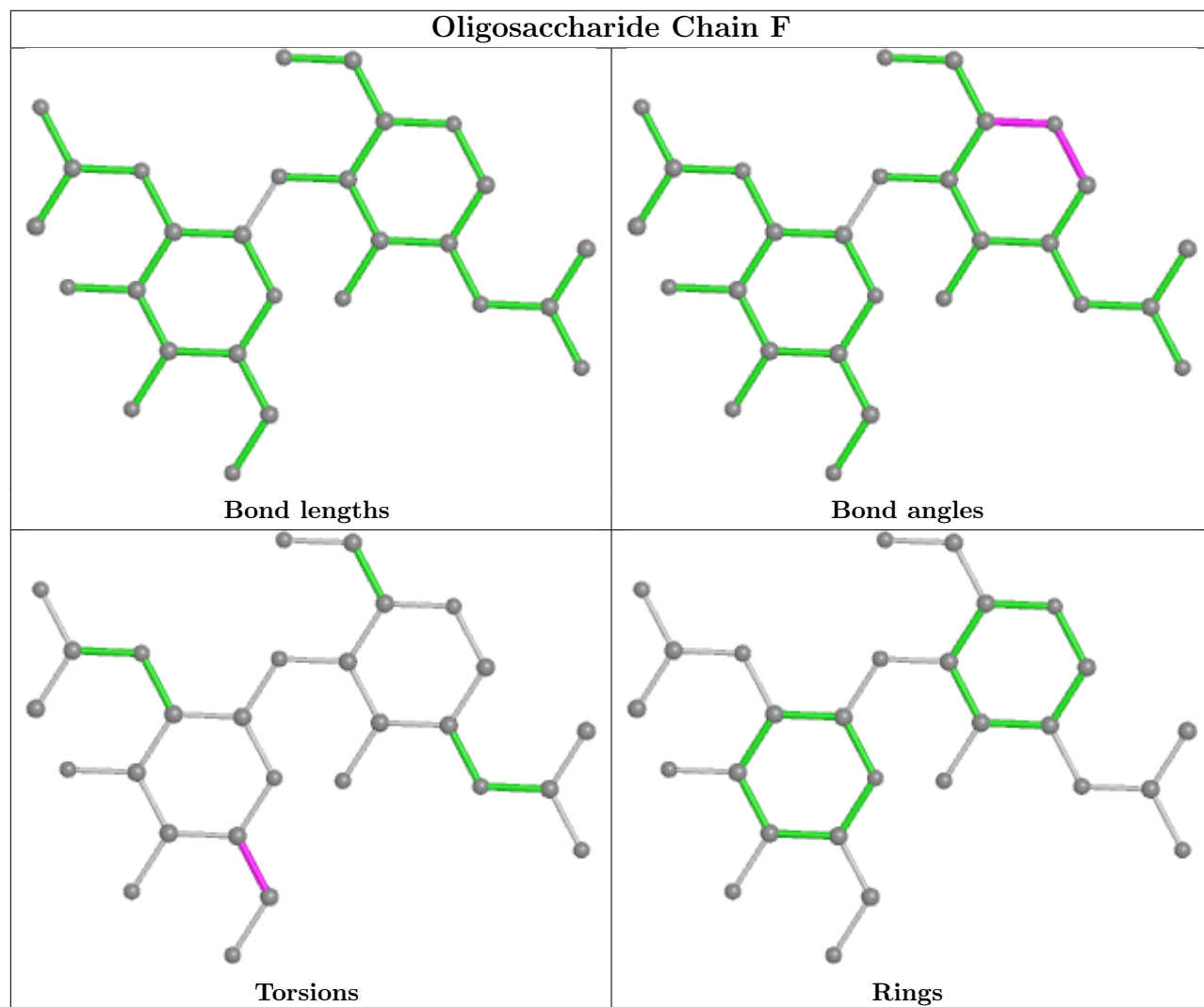
There are no ring outliers.

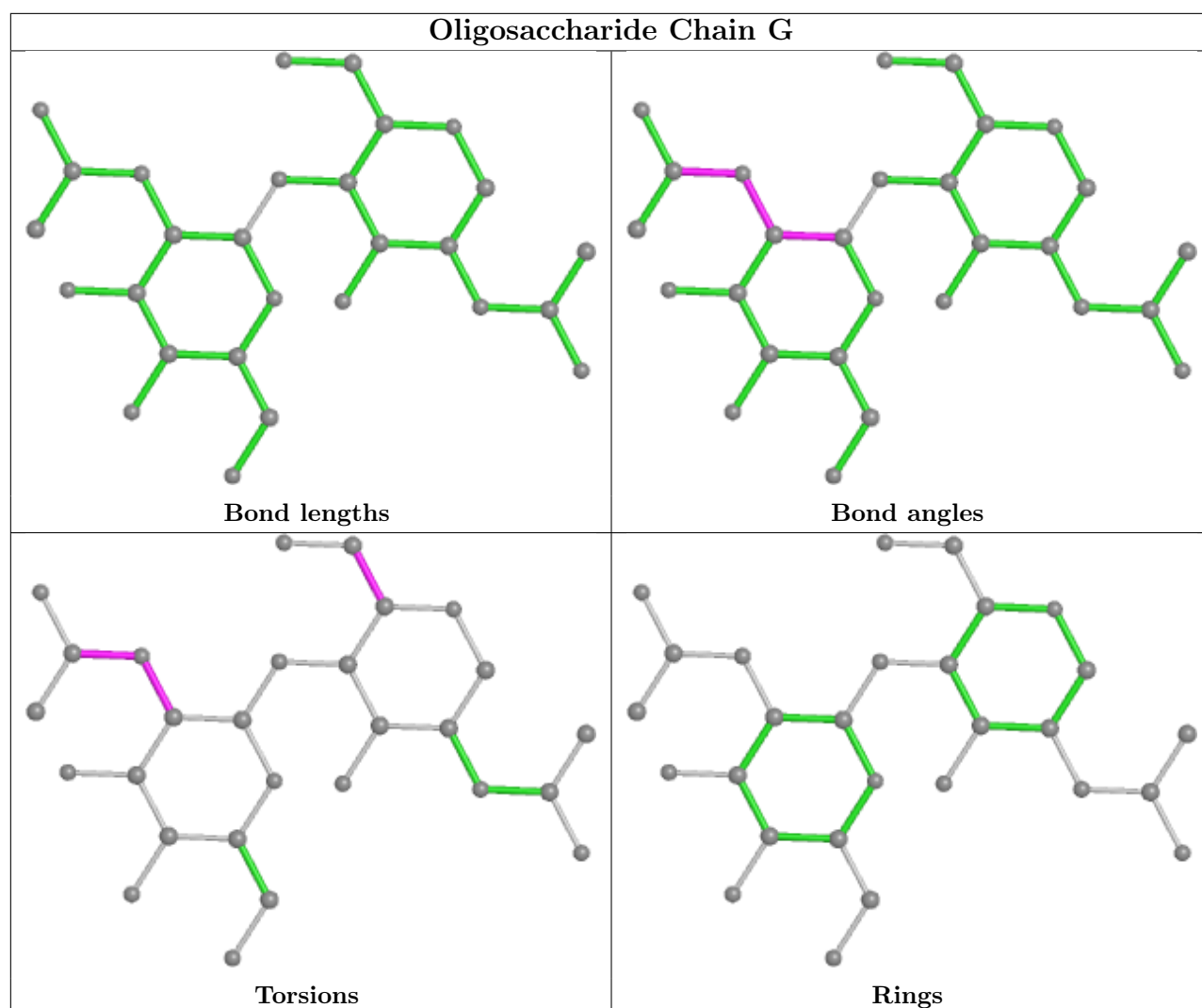
No monomer is involved in short contacts.

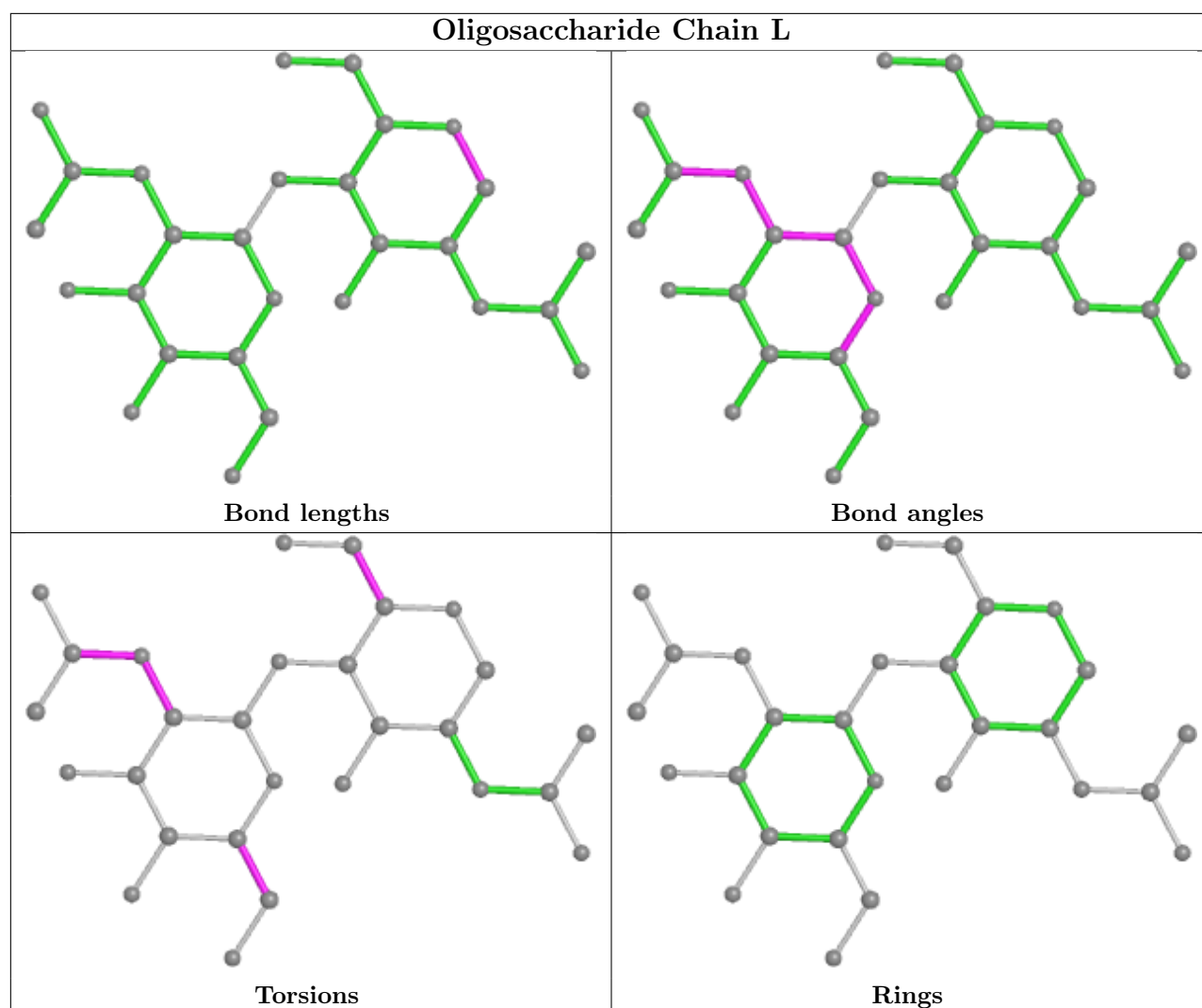
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

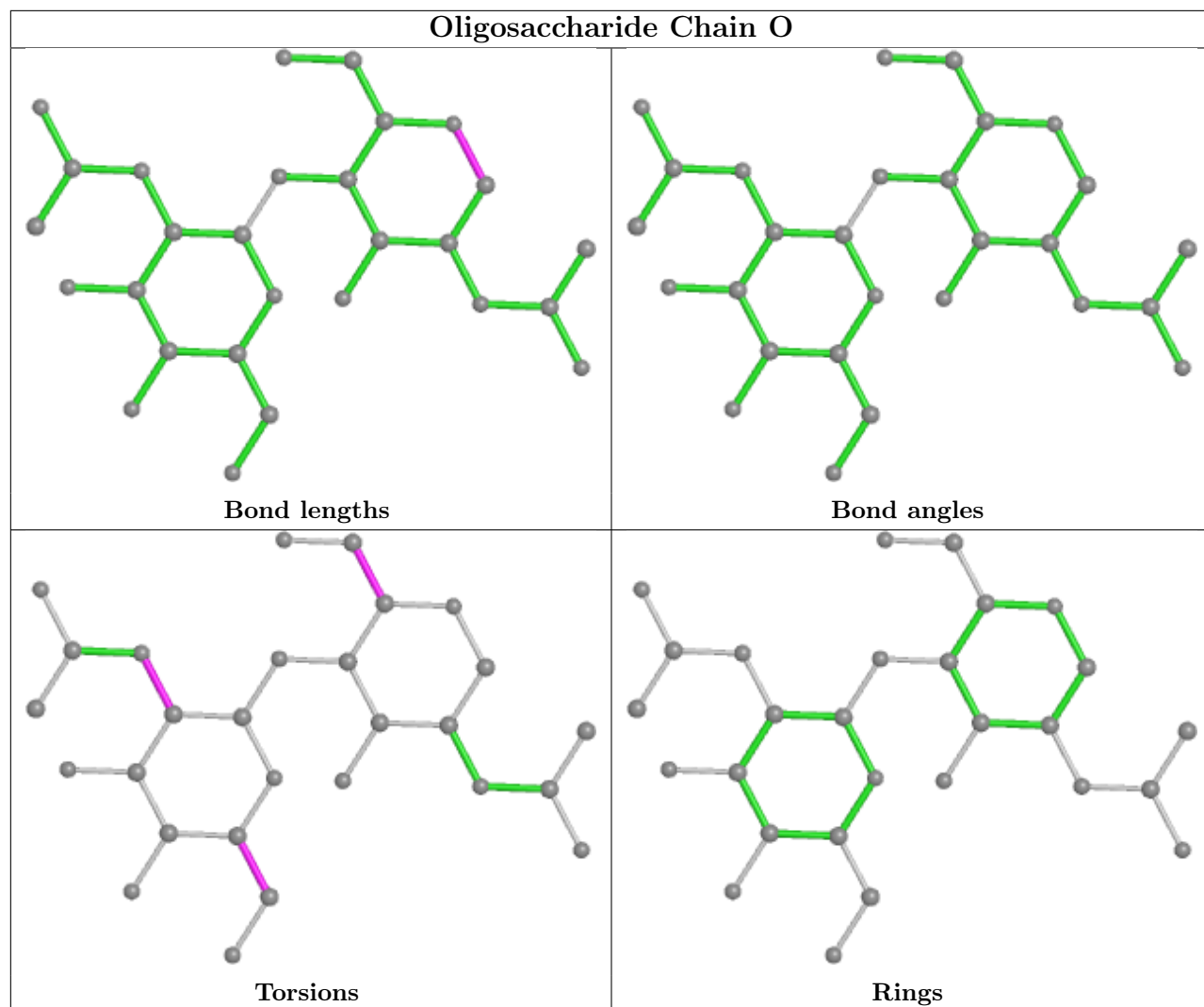


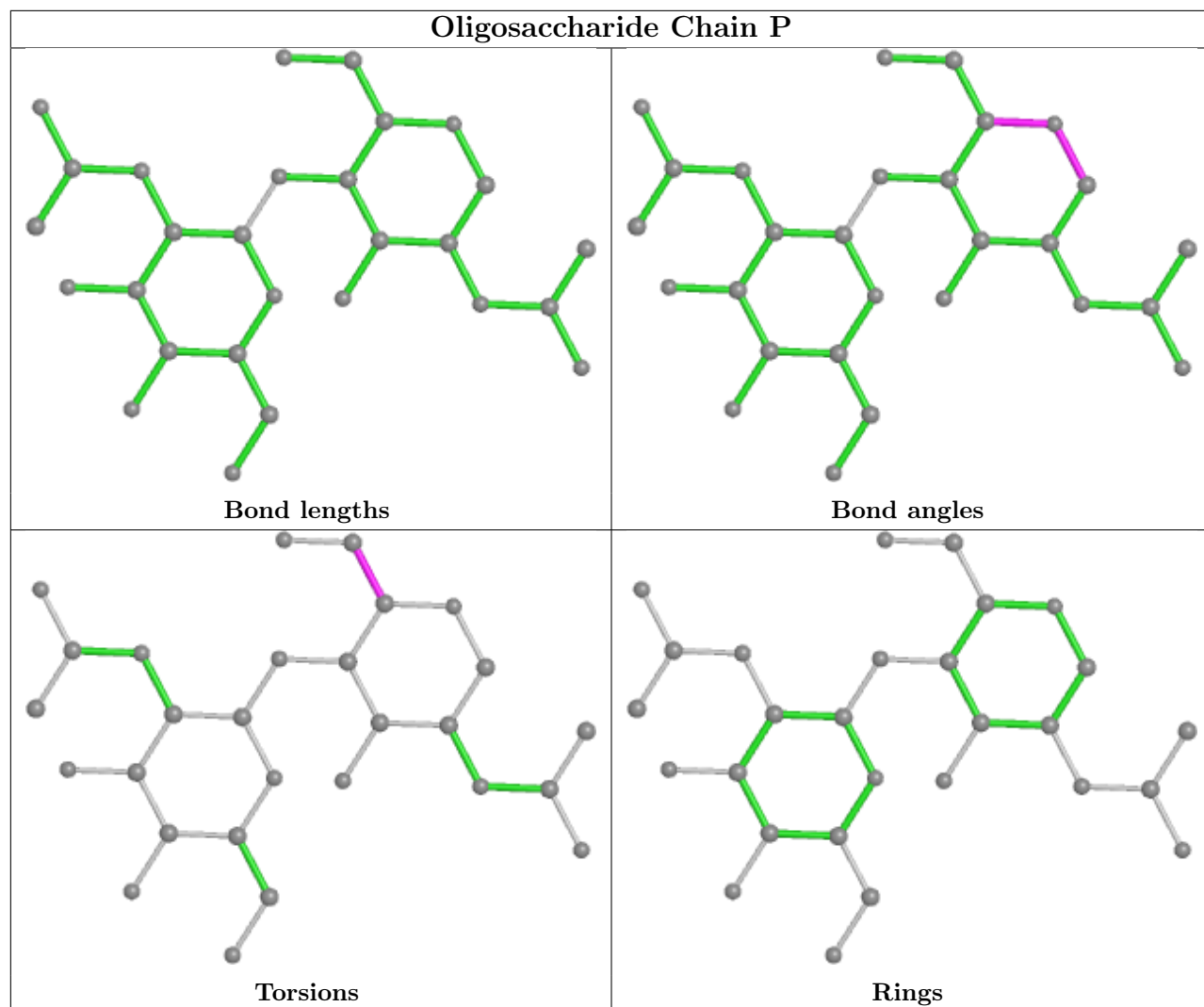


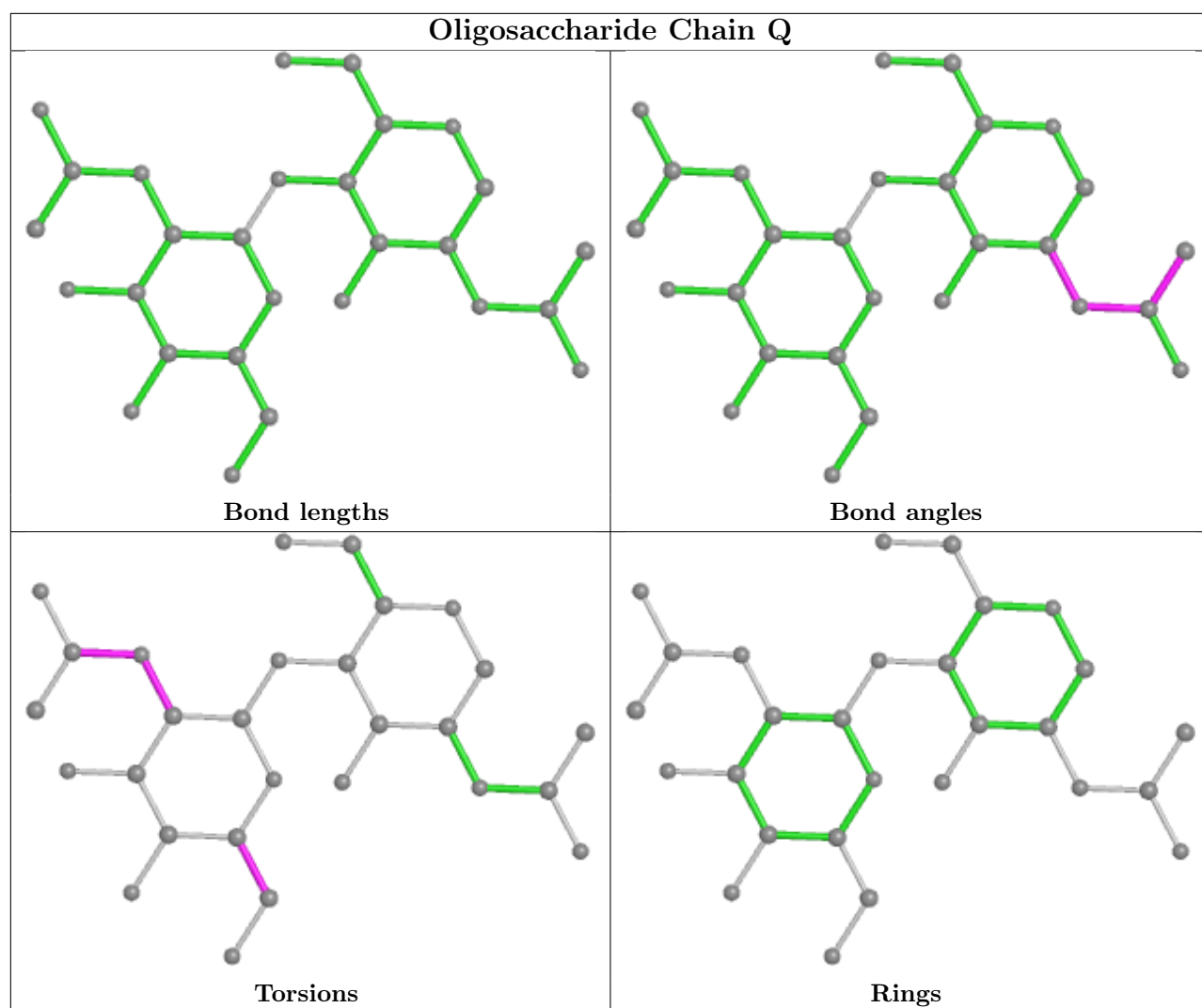


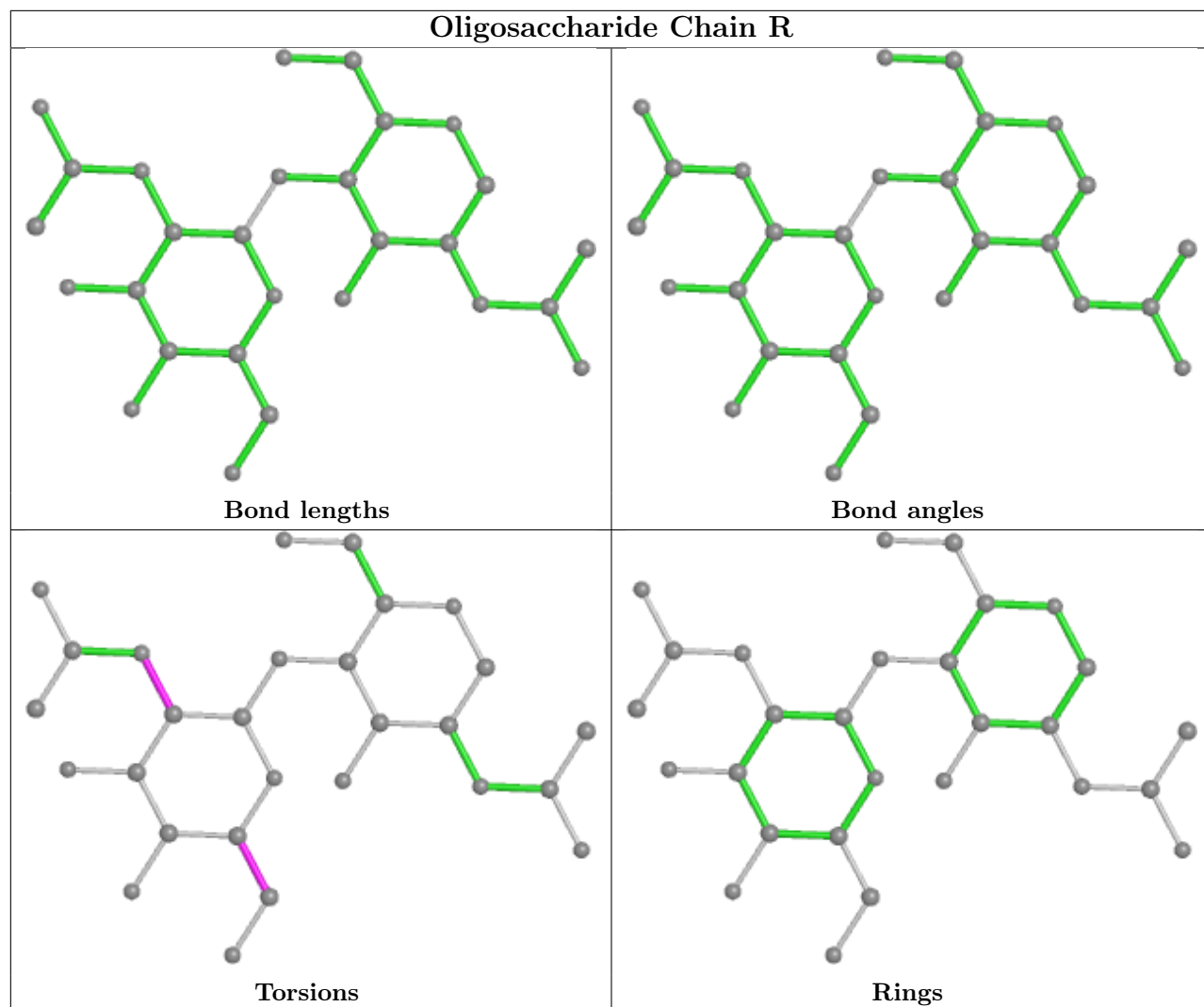


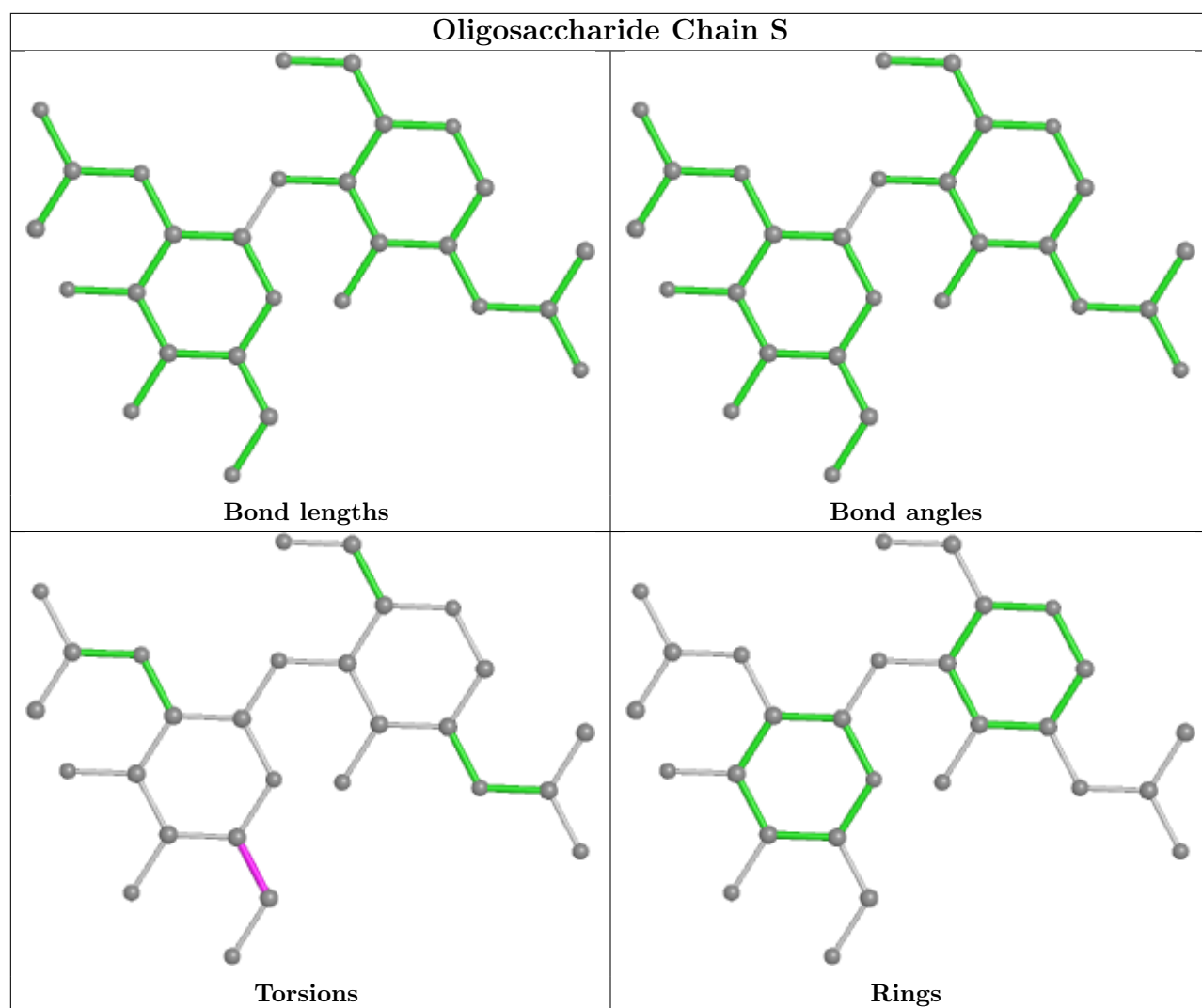


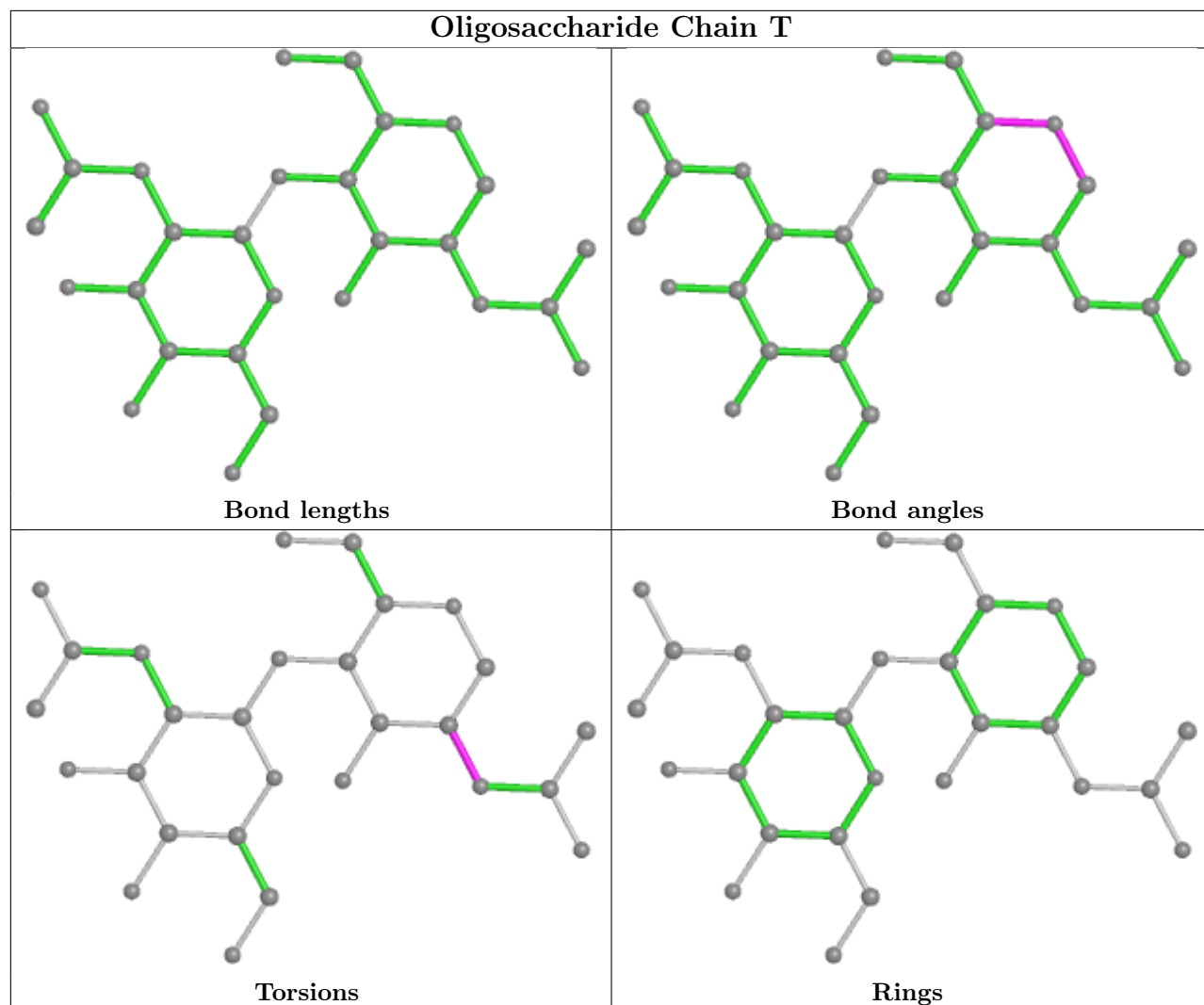


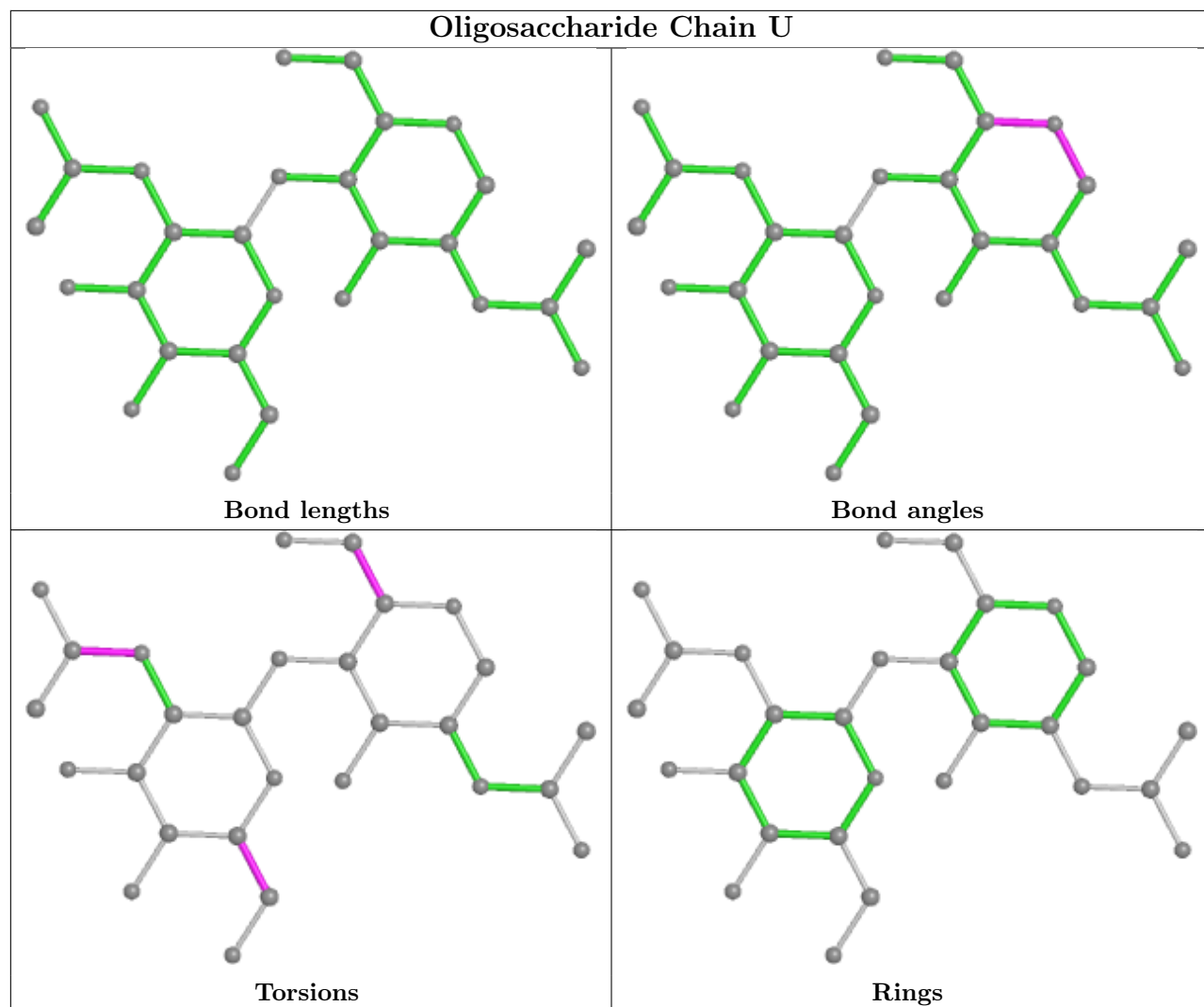


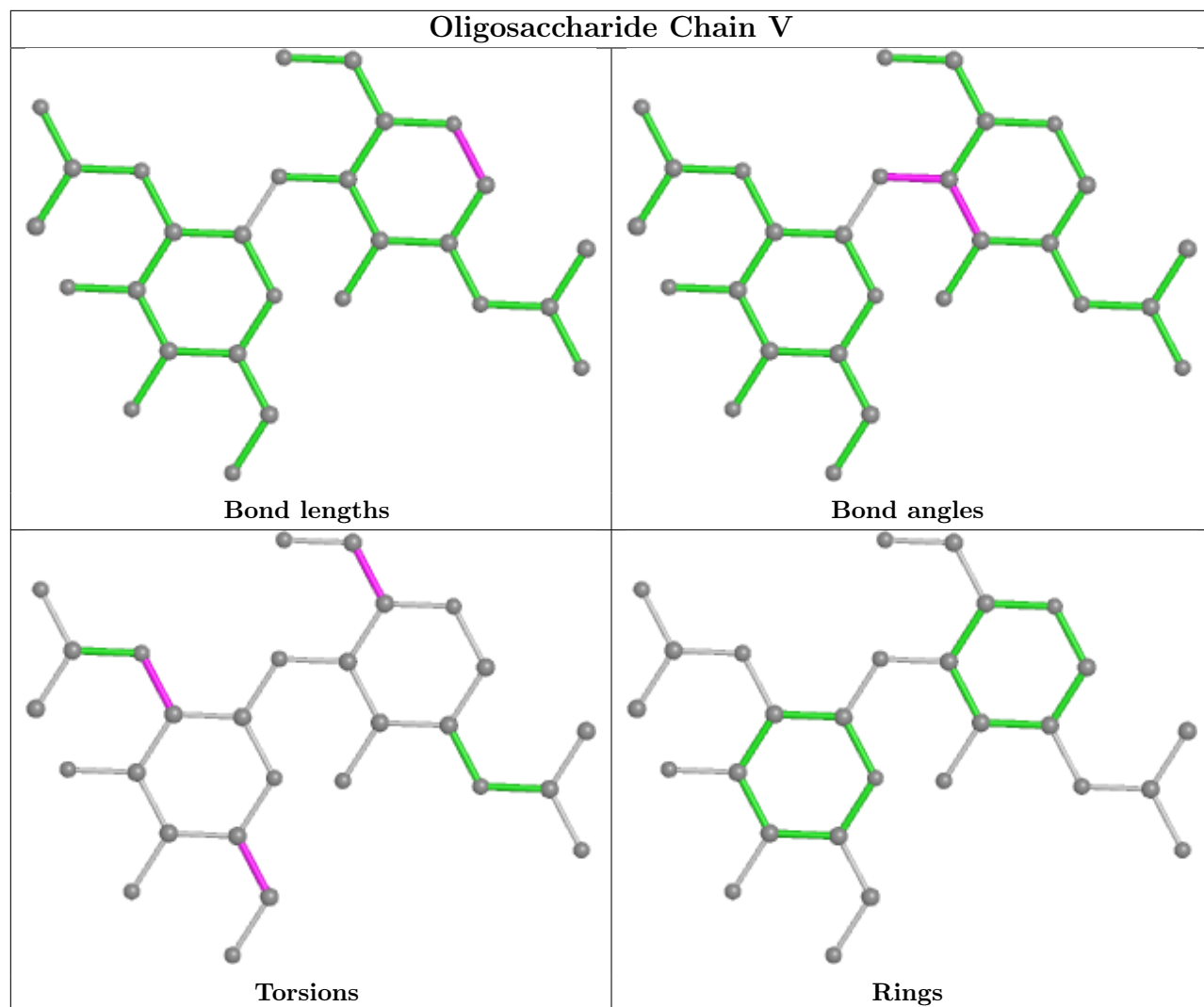


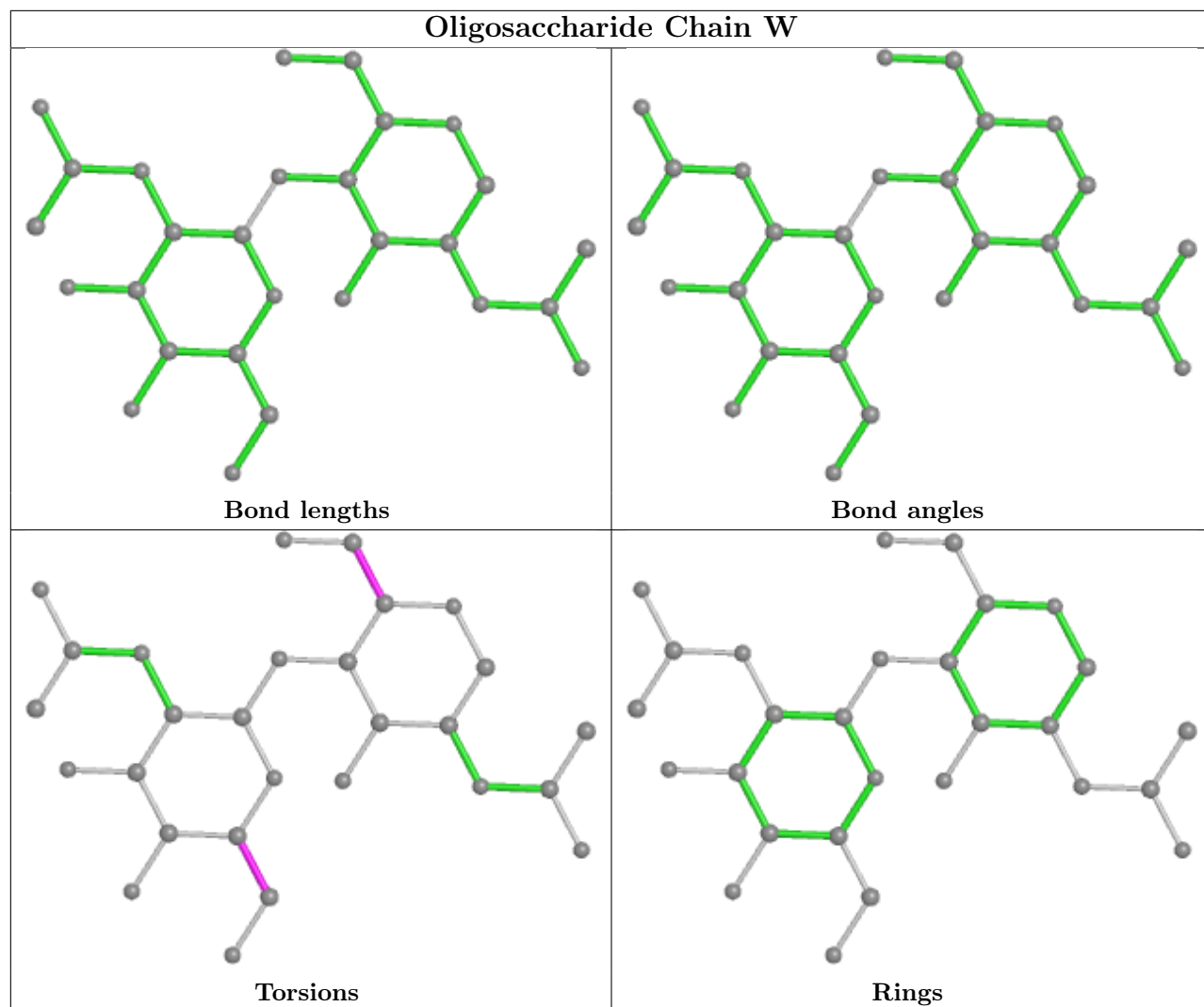


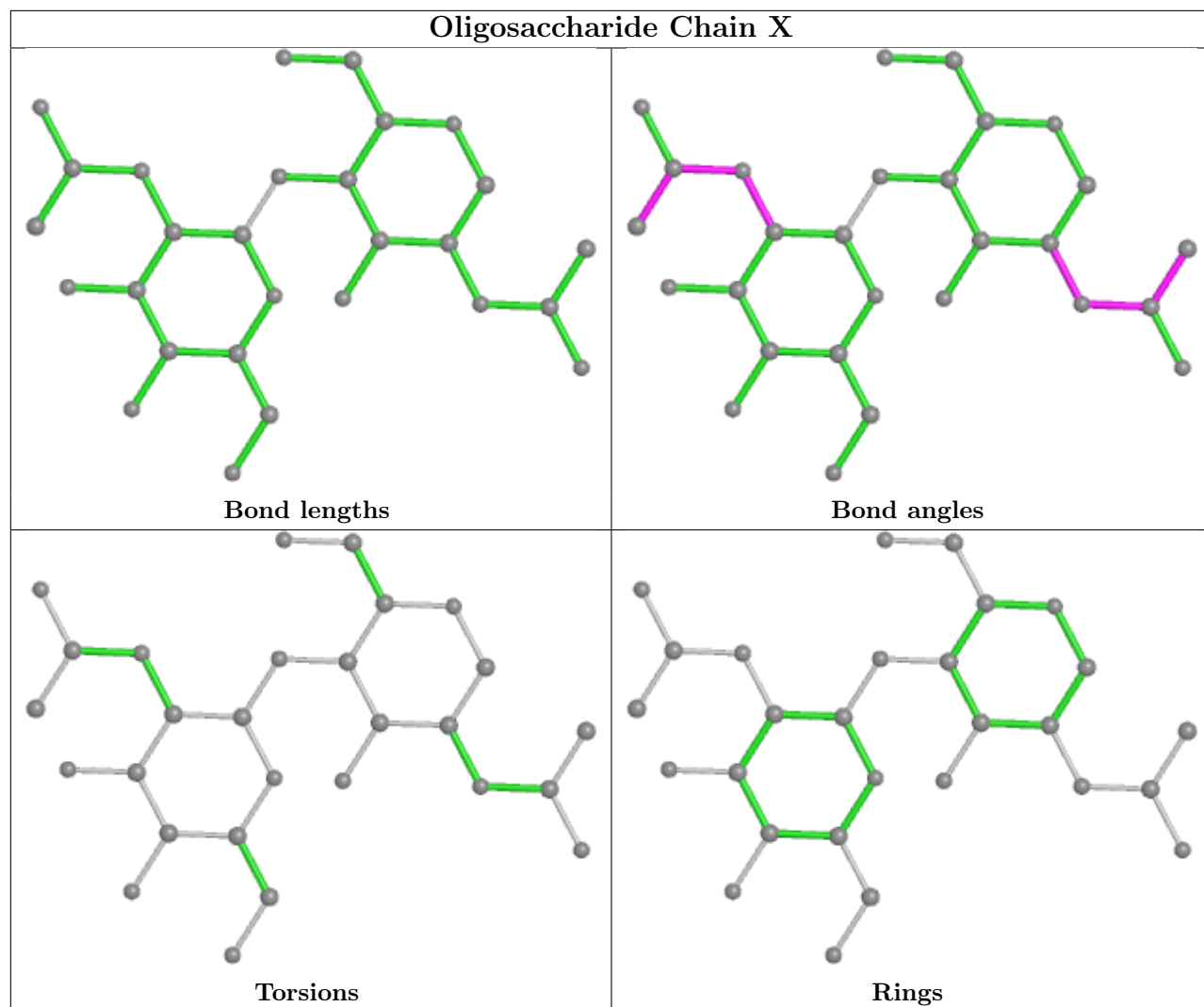


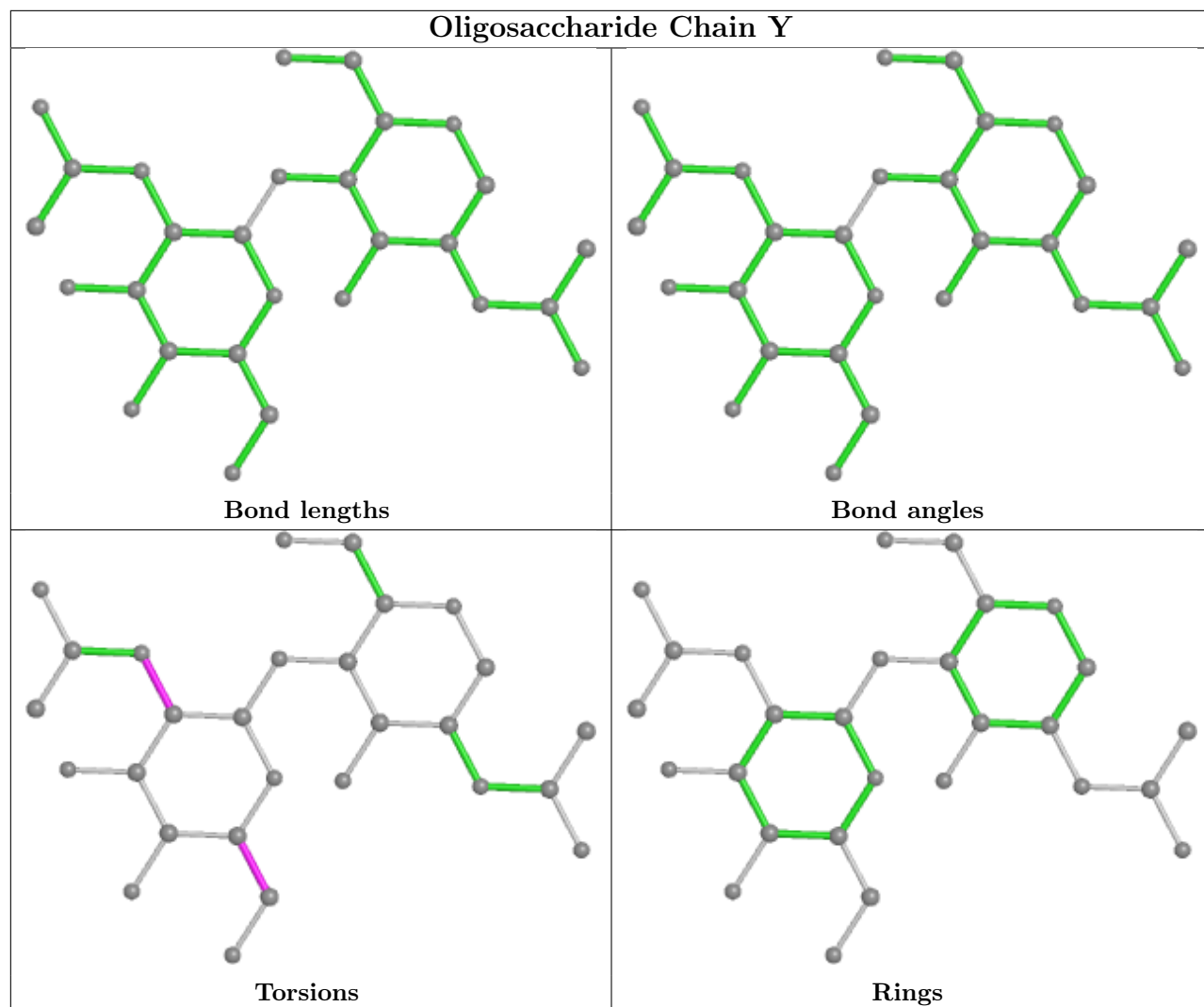


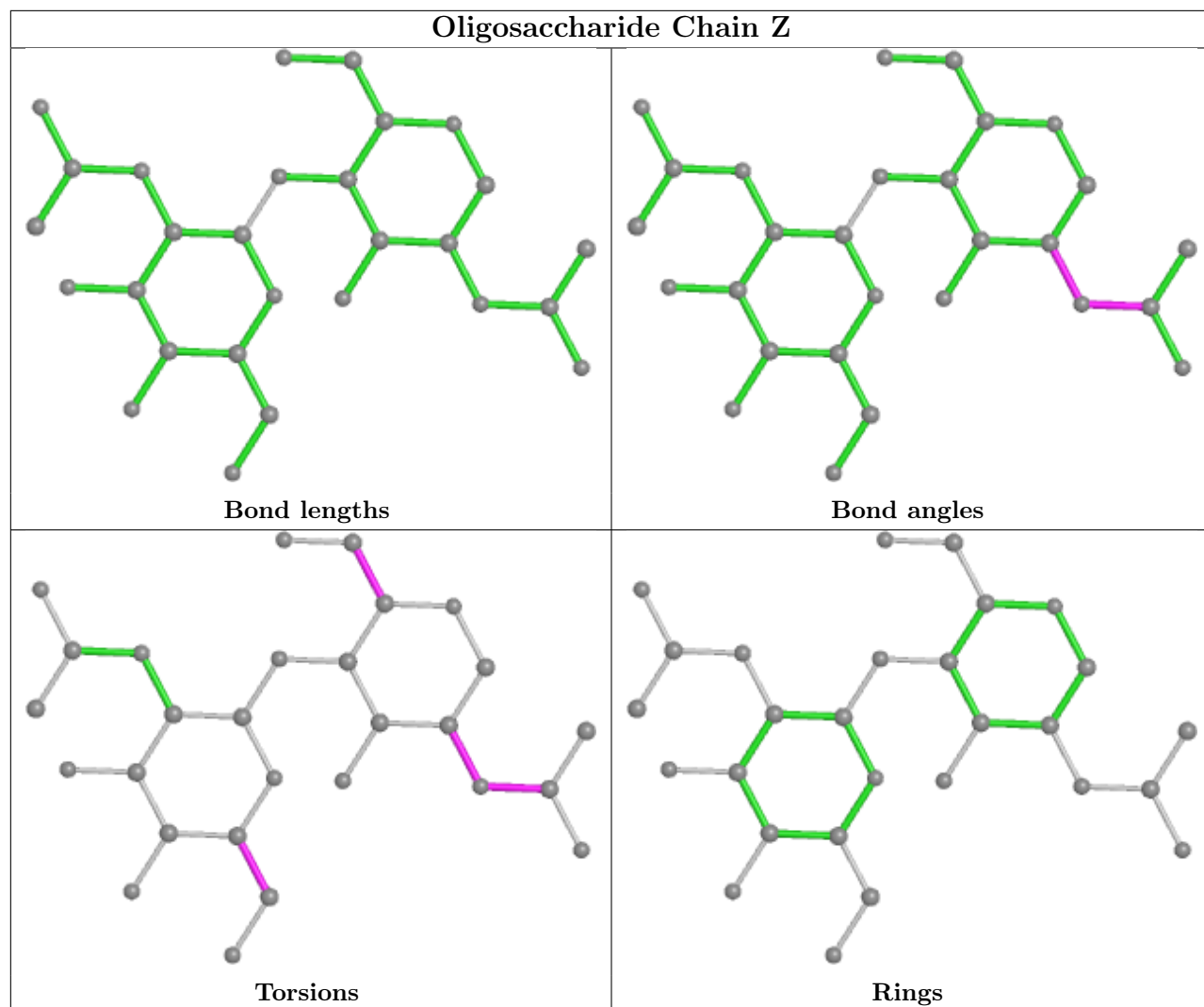


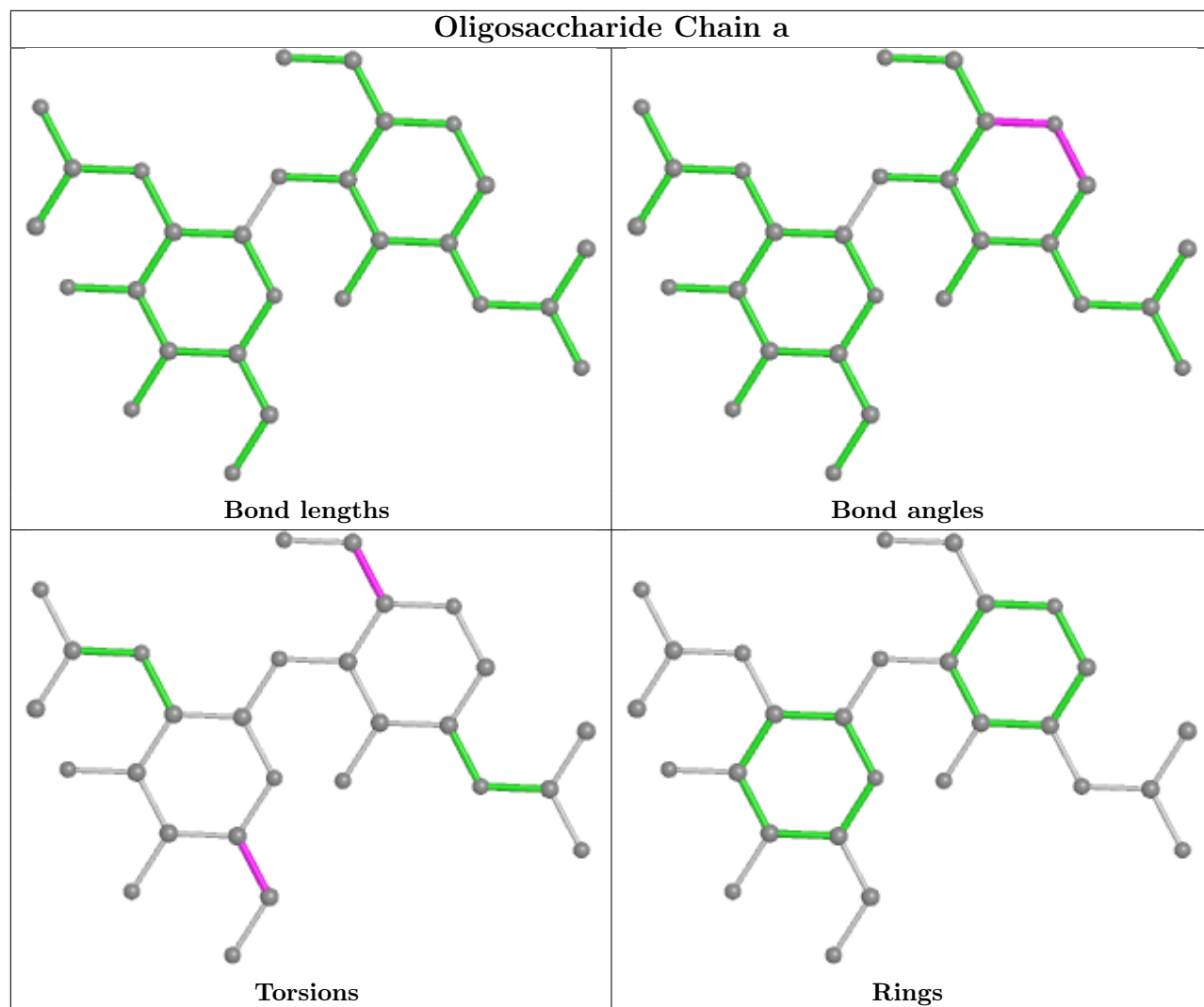


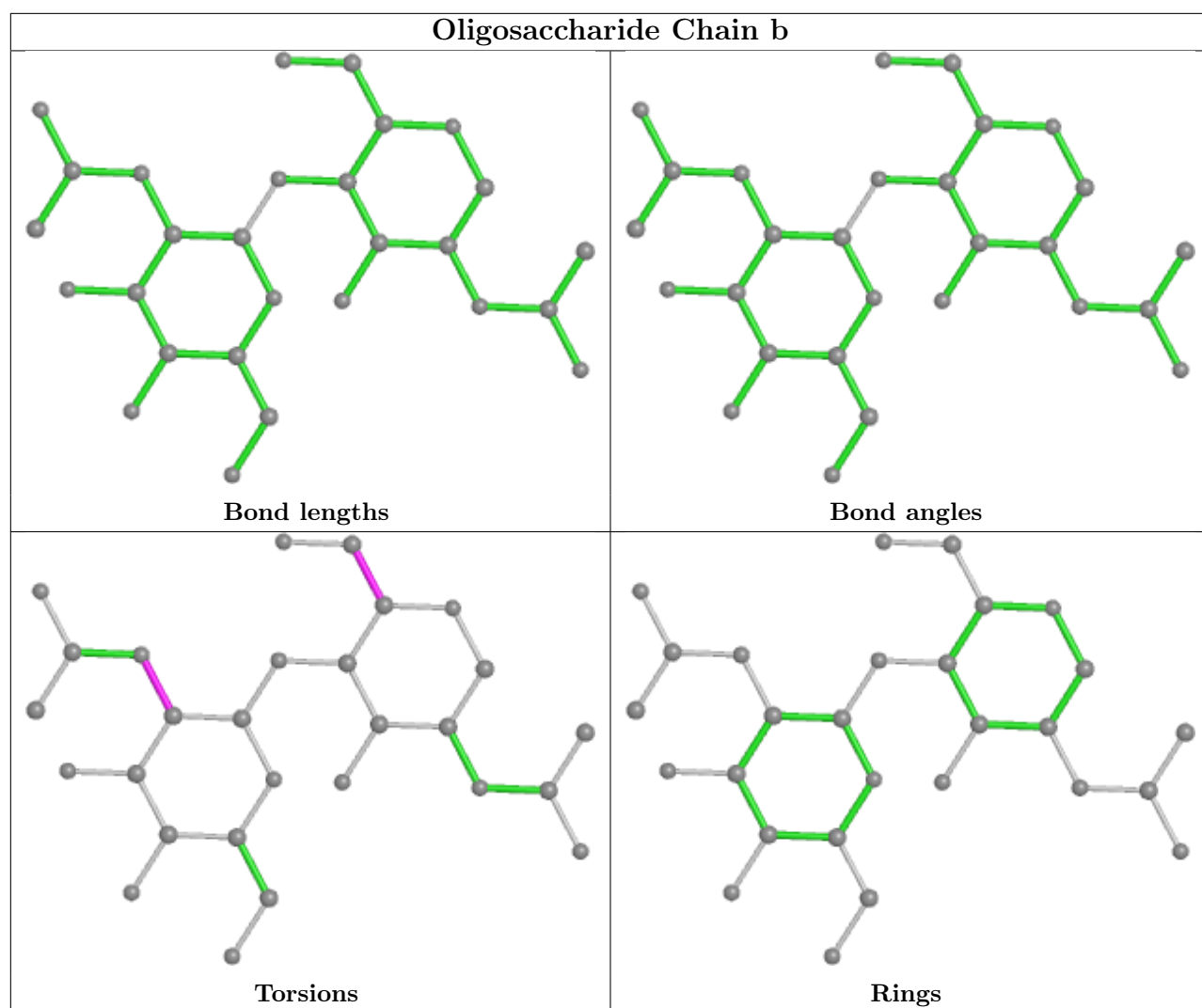


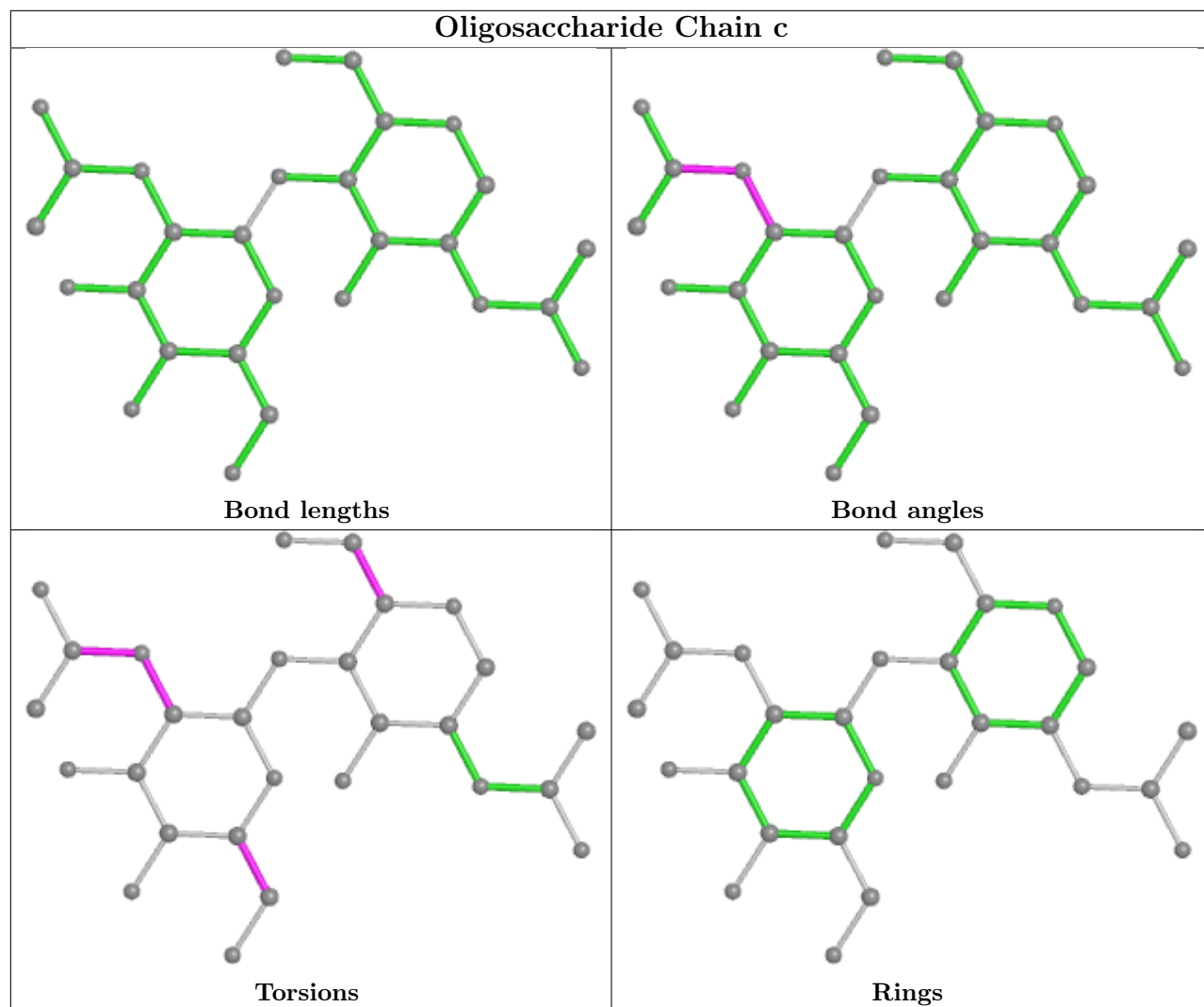


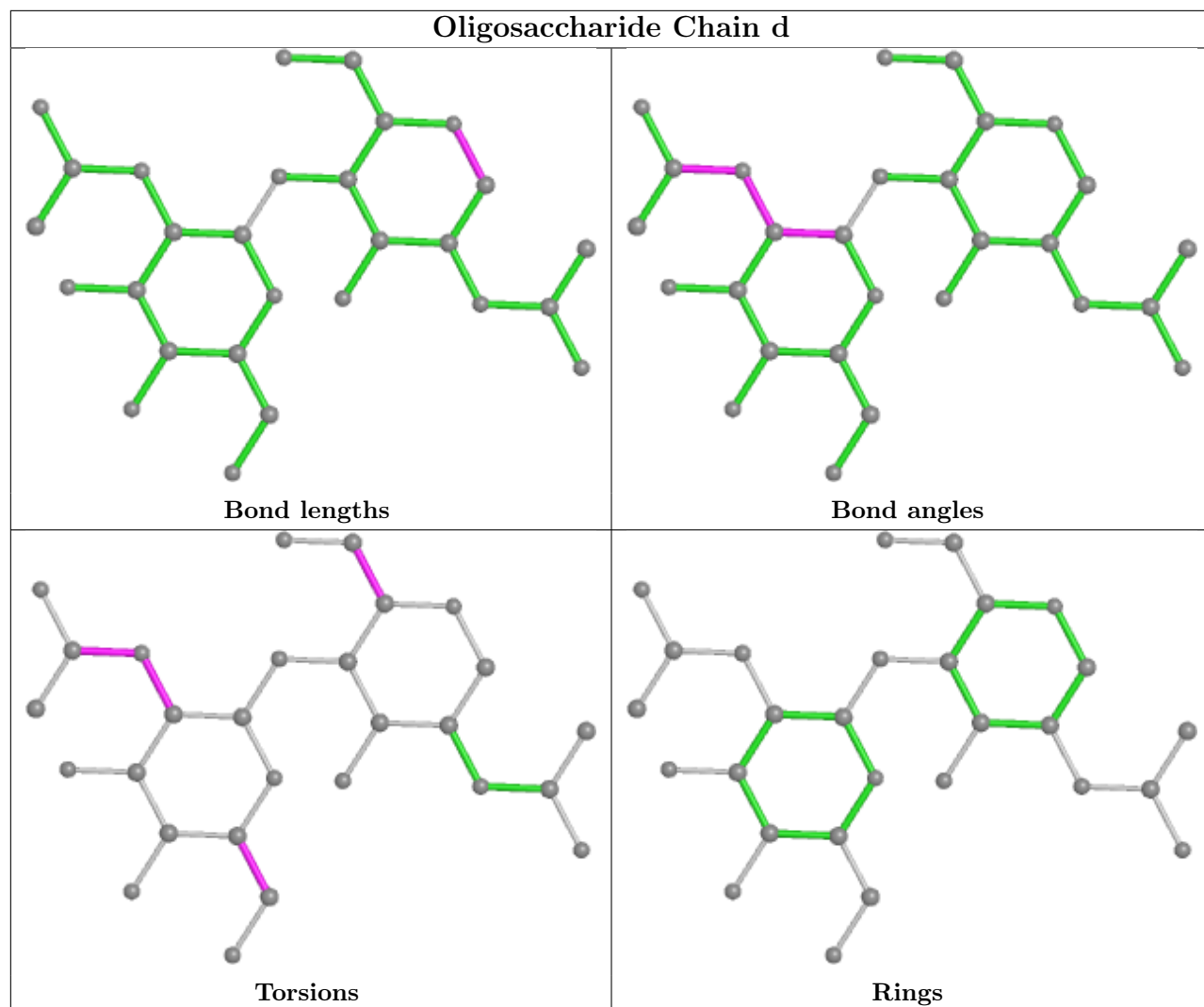


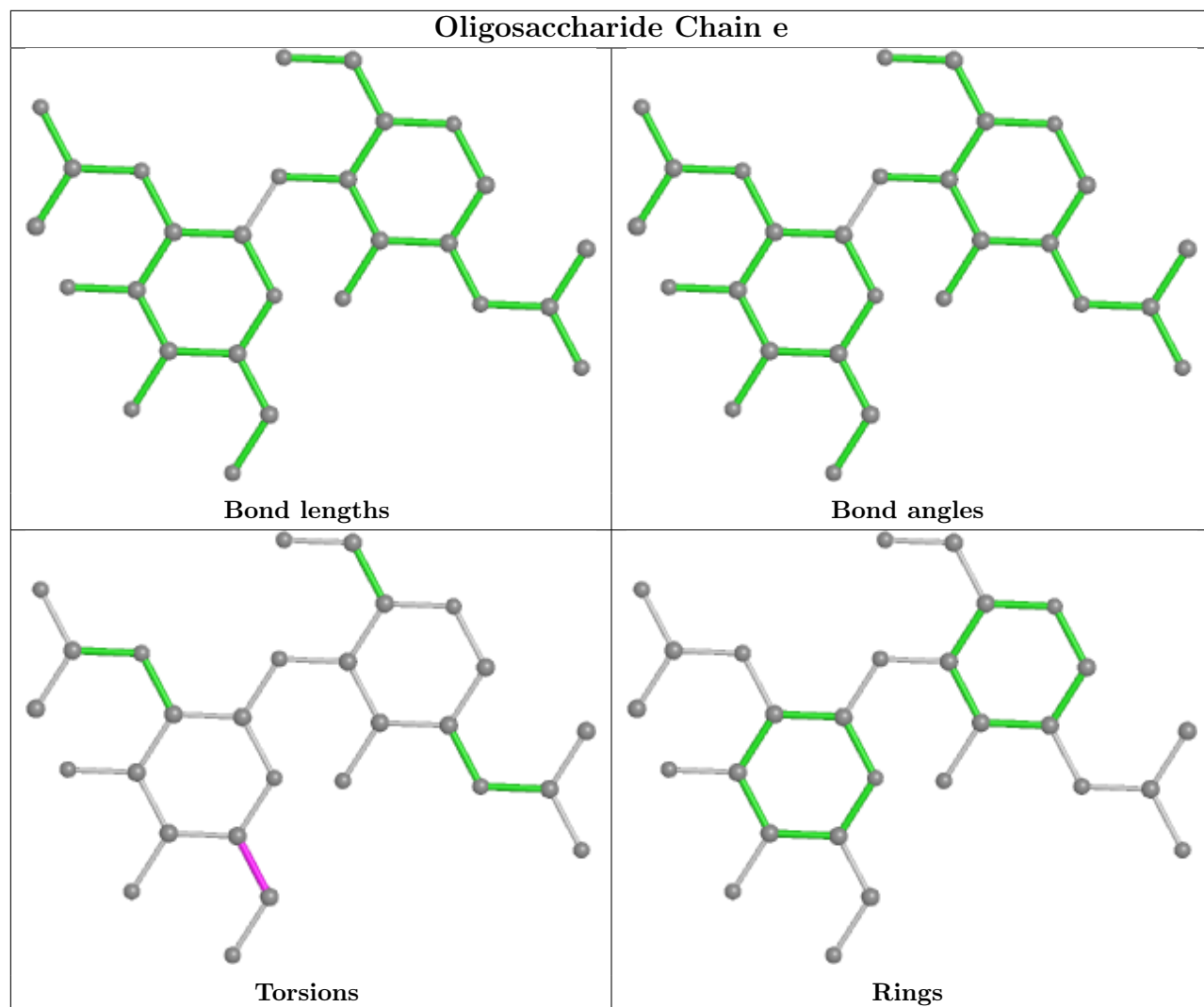


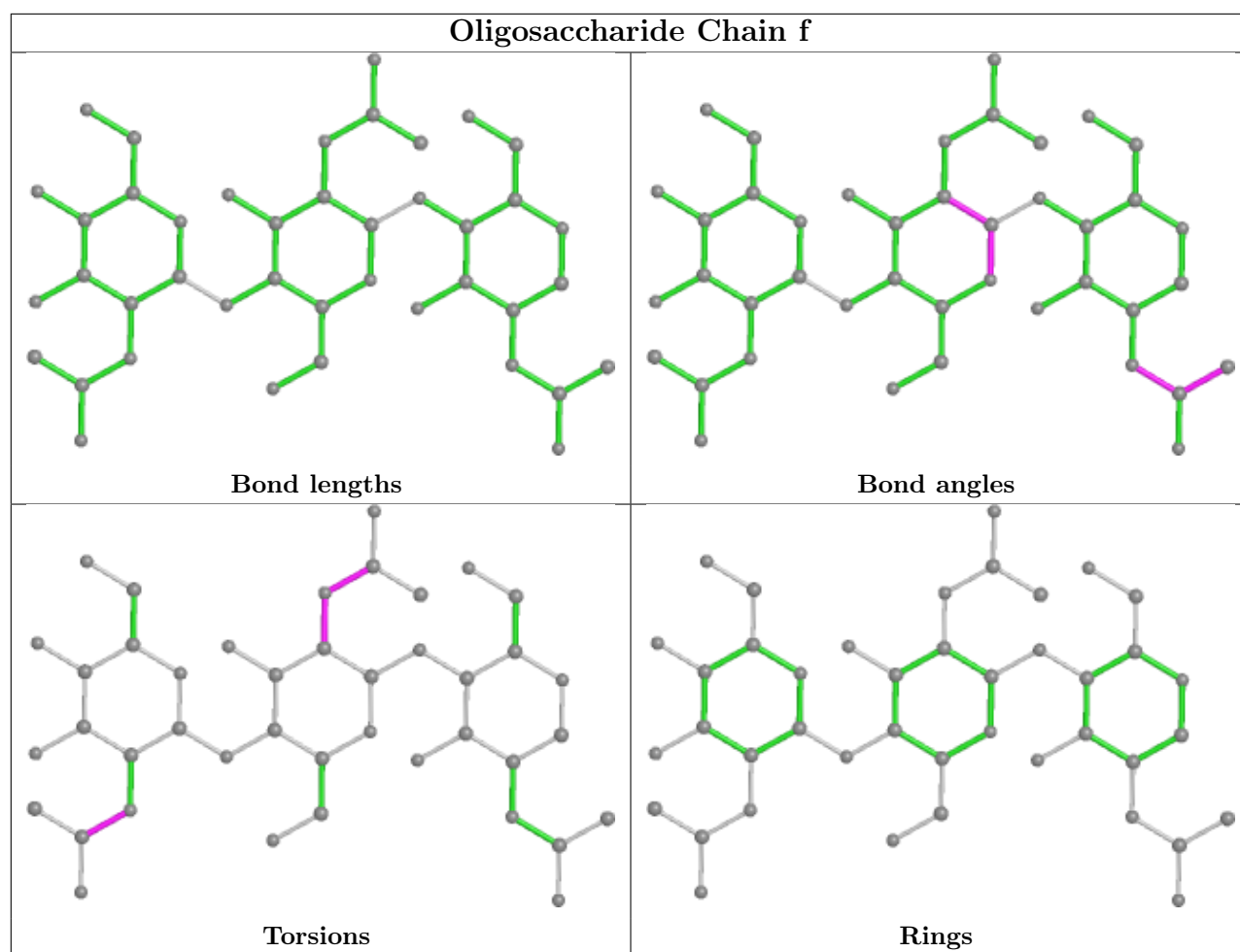


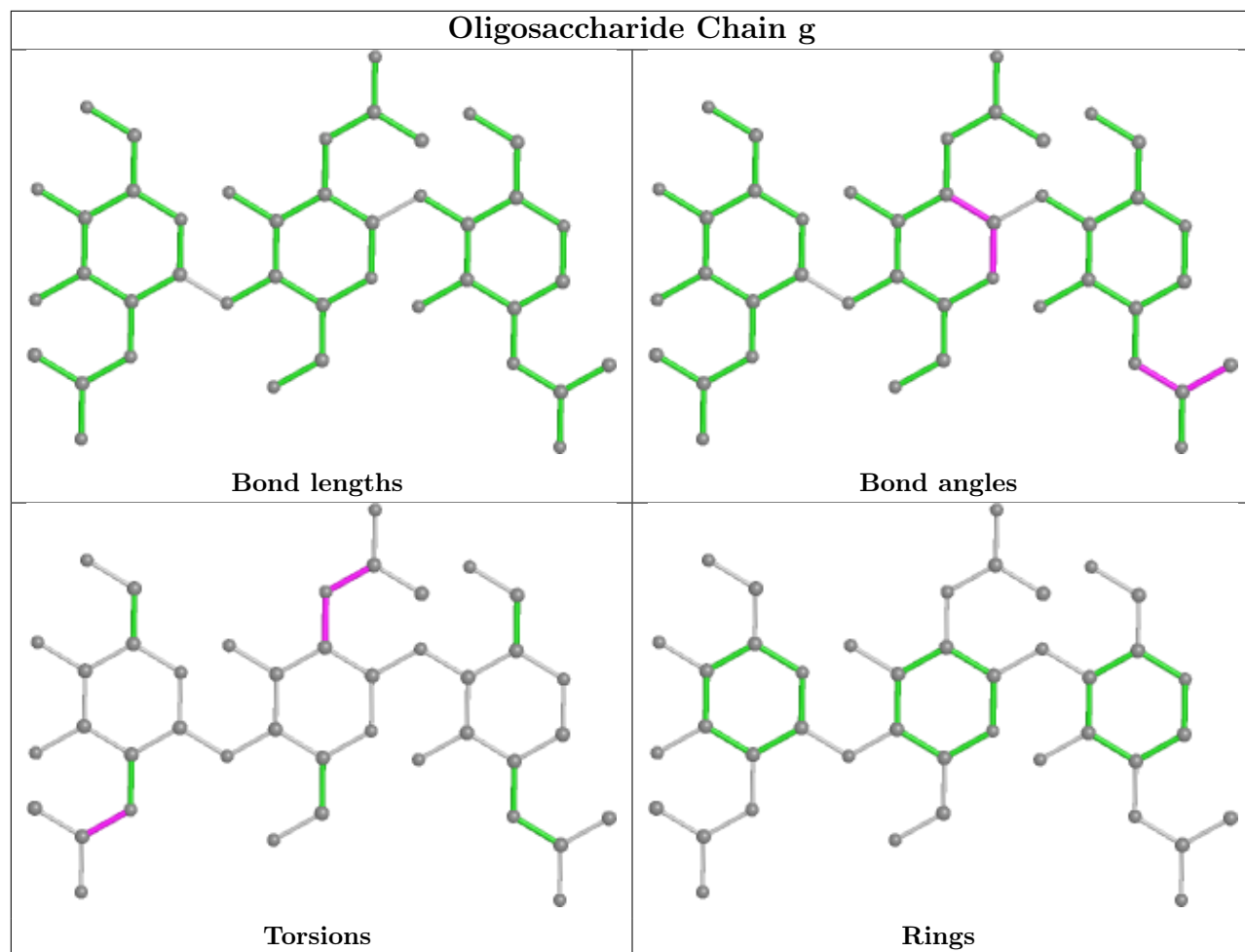


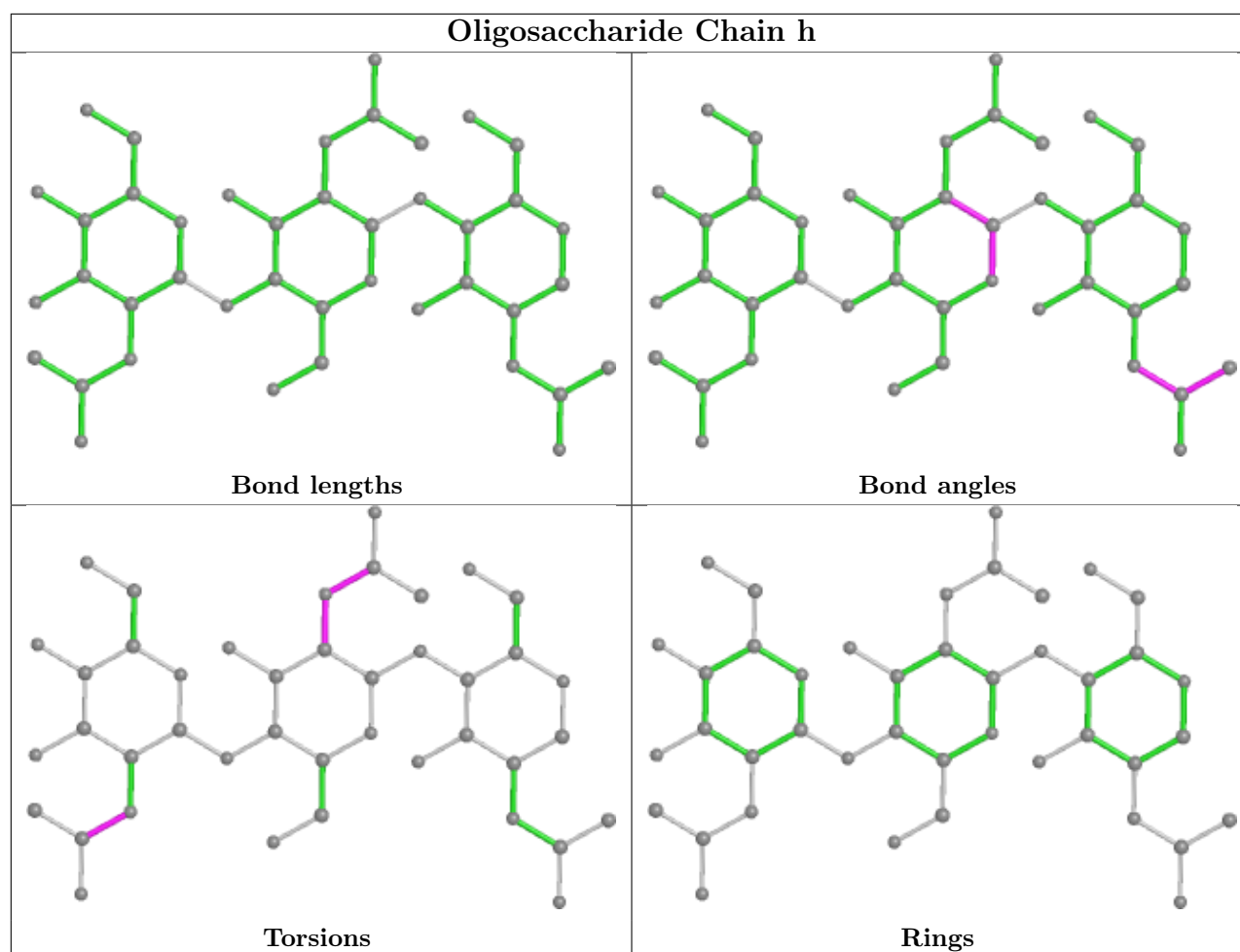












5.6 Ligand geometry [i](#)

27 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	$\# Z > 2$
6	NAG	B	1403	1	14,14,15	0.40	0	17,19,21	1.17	2 (11%)
6	NAG	B	1408	1	14,14,15	0.22	0	17,19,21	0.39	0
6	NAG	B	1406	1	14,14,15	0.43	0	17,19,21	0.73	1 (5%)
6	NAG	C	1403	1	14,14,15	0.55	0	17,19,21	0.44	0
6	NAG	A	1405	1	14,14,15	0.55	0	17,19,21	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1408	1	14,14,15	0.30	0	17,19,21	0.39	0
6	NAG	C	1405	1	14,14,15	0.39	0	17,19,21	1.29	2 (11%)
6	NAG	B	1407	1	14,14,15	0.33	0	17,19,21	0.40	0
6	NAG	B	1402	1	14,14,15	0.34	0	17,19,21	0.64	0
6	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
6	NAG	B	1409	1	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
6	NAG	B	1405	1	14,14,15	0.30	0	17,19,21	0.61	0
6	NAG	A	1407	1	14,14,15	0.26	0	17,19,21	0.49	0
6	NAG	C	1402	1	14,14,15	0.45	0	17,19,21	0.56	0
6	NAG	B	1401	1	14,14,15	0.32	0	17,19,21	0.55	0
6	NAG	B	1404	1	14,14,15	0.29	0	17,19,21	0.62	0
6	NAG	C	1404	1	14,14,15	0.30	0	17,19,21	0.62	0
6	NAG	A	1409	1	14,14,15	0.53	0	17,19,21	0.35	0
6	NAG	B	1410	-	14,14,15	0.33	0	17,19,21	0.42	0
6	NAG	A	1403	1	14,14,15	0.21	0	17,19,21	0.40	0
6	NAG	A	1402	1	14,14,15	0.22	0	17,19,21	0.62	0
6	NAG	C	1408	1	14,14,15	0.15	0	17,19,21	0.57	0
6	NAG	C	1401	1	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
6	NAG	C	1406	1	14,14,15	0.20	0	17,19,21	0.37	0
6	NAG	A	1404	1	14,14,15	0.44	0	17,19,21	0.55	0
6	NAG	A	1401	1	14,14,15	0.29	0	17,19,21	0.34	0
6	NAG	C	1407	1	14,14,15	0.33	0	17,19,21	0.63	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
6	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1406	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1403	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
6	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1405	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1407	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1409	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1410	-	-	0/6/23/26	0/1/1/1
6	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1407	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1405	NAG	C2-N2-C7	4.34	129.09	122.90
6	C	1405	NAG	C2-N2-C7	4.33	129.06	122.90
6	C	1401	NAG	C1-O5-C5	2.86	116.06	112.19
6	B	1406	NAG	C1-O5-C5	2.36	115.38	112.19
6	B	1409	NAG	C8-C7-N2	2.31	120.01	116.10
6	B	1403	NAG	C8-C7-N2	2.26	119.93	116.10
6	C	1405	NAG	C1-C2-N2	2.22	114.27	110.49
6	B	1403	NAG	C2-N2-C7	-2.13	119.87	122.90
6	B	1409	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1405	NAG	C8-C7-N2-C2
6	B	1405	NAG	O7-C7-N2-C2
6	B	1407	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	B	1401	NAG	O5-C5-C6-O6
6	A	1406	NAG	O5-C5-C6-O6
6	B	1402	NAG	O5-C5-C6-O6
6	C	1404	NAG	O5-C5-C6-O6
6	C	1408	NAG	O5-C5-C6-O6
6	A	1402	NAG	C4-C5-C6-O6
6	A	1401	NAG	O5-C5-C6-O6
6	A	1402	NAG	O5-C5-C6-O6
6	A	1404	NAG	O5-C5-C6-O6
6	B	1401	NAG	C4-C5-C6-O6
6	A	1405	NAG	O5-C5-C6-O6
6	B	1404	NAG	O5-C5-C6-O6
6	A	1408	NAG	O5-C5-C6-O6
6	A	1409	NAG	C4-C5-C6-O6
6	B	1407	NAG	C4-C5-C6-O6
6	B	1402	NAG	C4-C5-C6-O6
6	B	1406	NAG	O5-C5-C6-O6
6	A	1405	NAG	C4-C5-C6-O6
6	A	1405	NAG	C8-C7-N2-C2
6	A	1405	NAG	O7-C7-N2-C2
6	C	1405	NAG	C8-C7-N2-C2
6	C	1405	NAG	O7-C7-N2-C2
6	C	1406	NAG	C8-C7-N2-C2
6	C	1406	NAG	O7-C7-N2-C2
6	B	1404	NAG	C4-C5-C6-O6
6	C	1404	NAG	C4-C5-C6-O6
6	A	1409	NAG	O5-C5-C6-O6
6	A	1406	NAG	C4-C5-C6-O6
6	B	1406	NAG	C4-C5-C6-O6
6	C	1401	NAG	O5-C5-C6-O6
6	C	1408	NAG	C4-C5-C6-O6
6	A	1404	NAG	C4-C5-C6-O6
6	C	1407	NAG	C4-C5-C6-O6
6	A	1403	NAG	O5-C5-C6-O6
6	C	1403	NAG	O5-C5-C6-O6
6	A	1403	NAG	C4-C5-C6-O6
6	B	1408	NAG	C4-C5-C6-O6
6	C	1403	NAG	C4-C5-C6-O6
6	C	1403	NAG	C1-C2-N2-C7
6	A	1408	NAG	C4-C5-C6-O6
6	C	1407	NAG	O5-C5-C6-O6
6	B	1408	NAG	O5-C5-C6-O6

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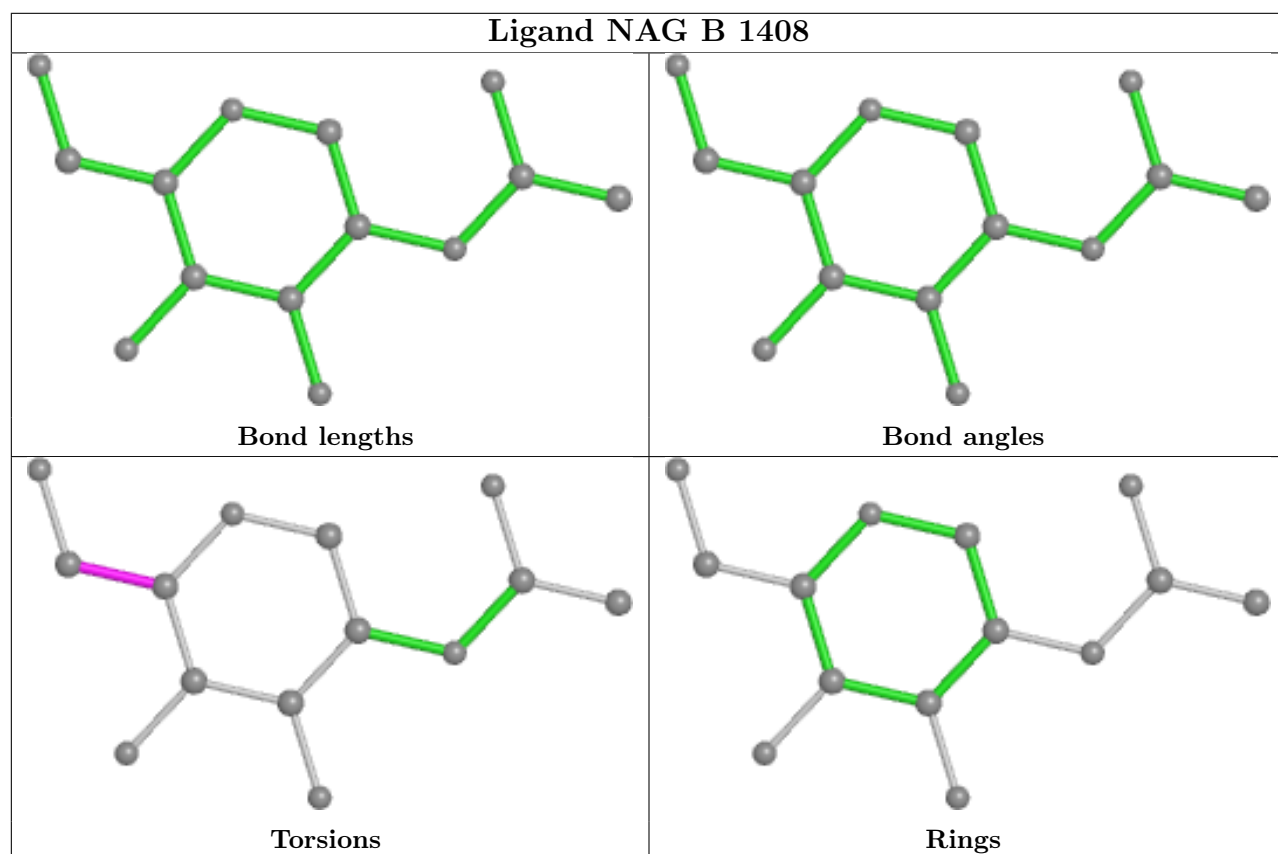
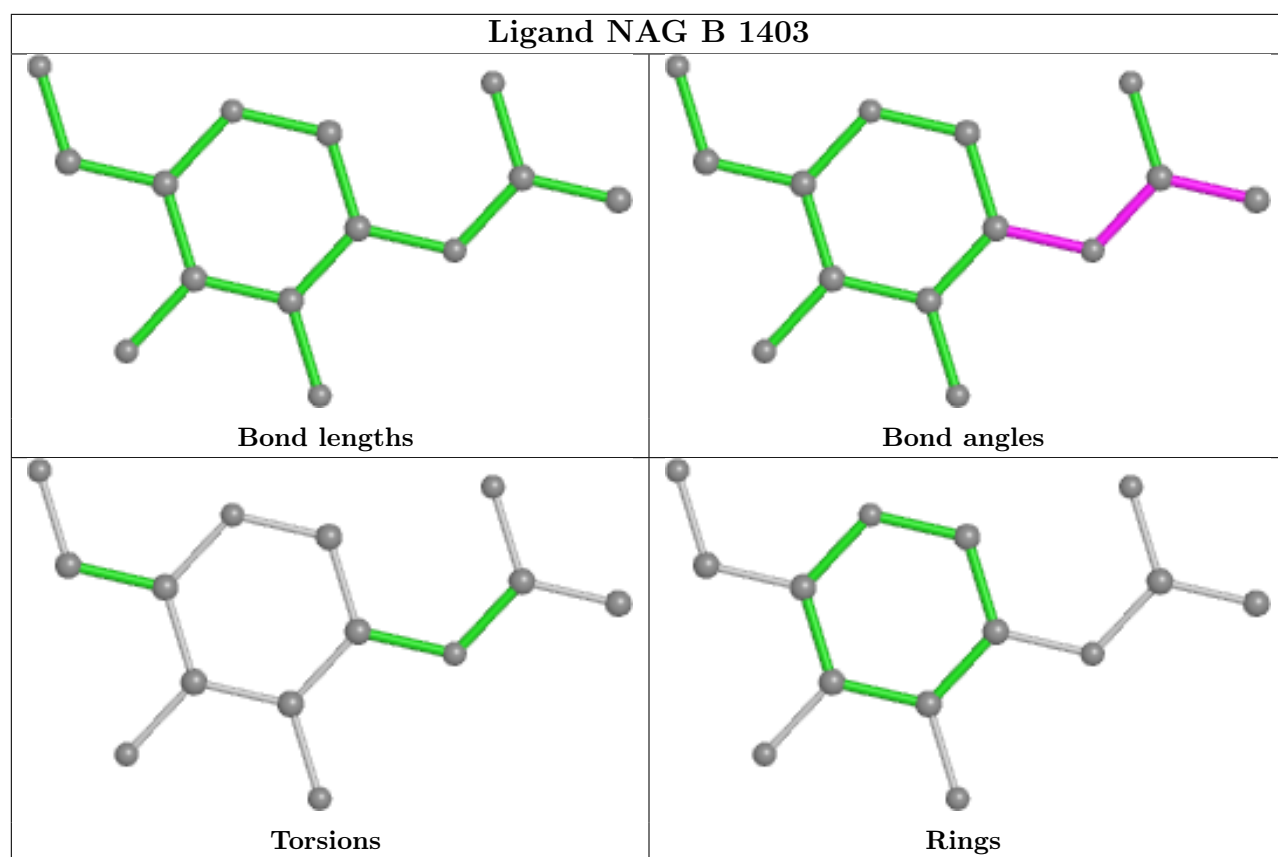
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Mol	Chain	Res	Type	Atoms
6	A	1401	NAG	C4-C5-C6-O6
6	A	1407	NAG	C1-C2-N2-C7
6	B	1406	NAG	C3-C2-N2-C7
6	C	1407	NAG	C3-C2-N2-C7
6	A	1405	NAG	C3-C2-N2-C7
6	C	1403	NAG	C3-C2-N2-C7
6	C	1405	NAG	C3-C2-N2-C7

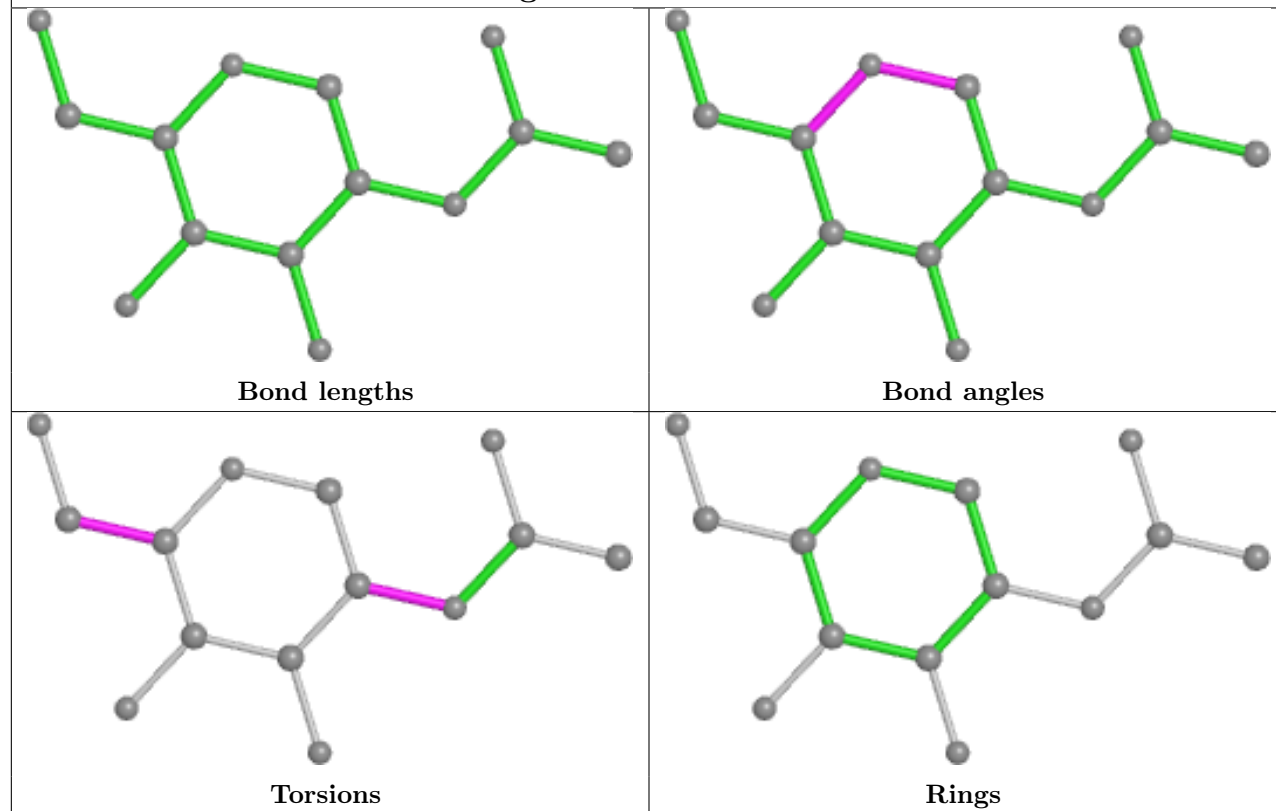
There are no ring outliers.

No monomer is involved in short contacts.

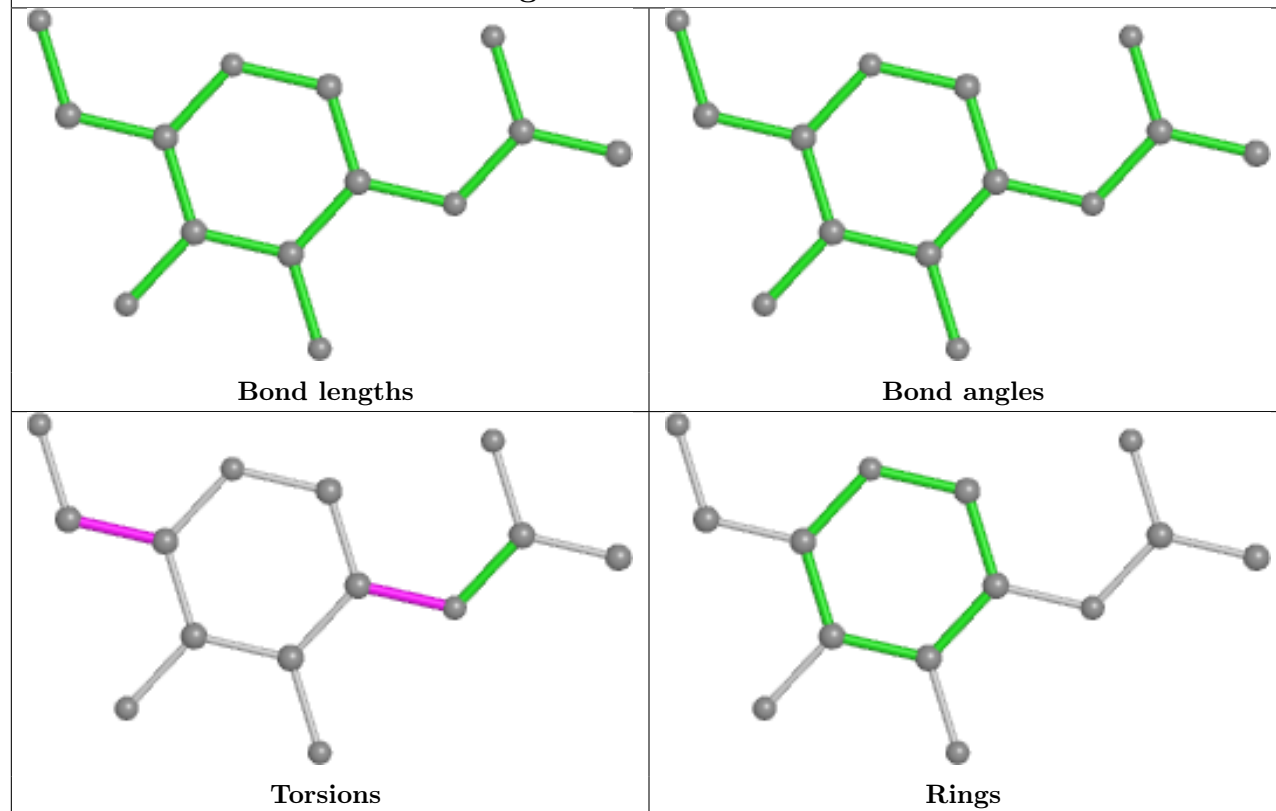
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



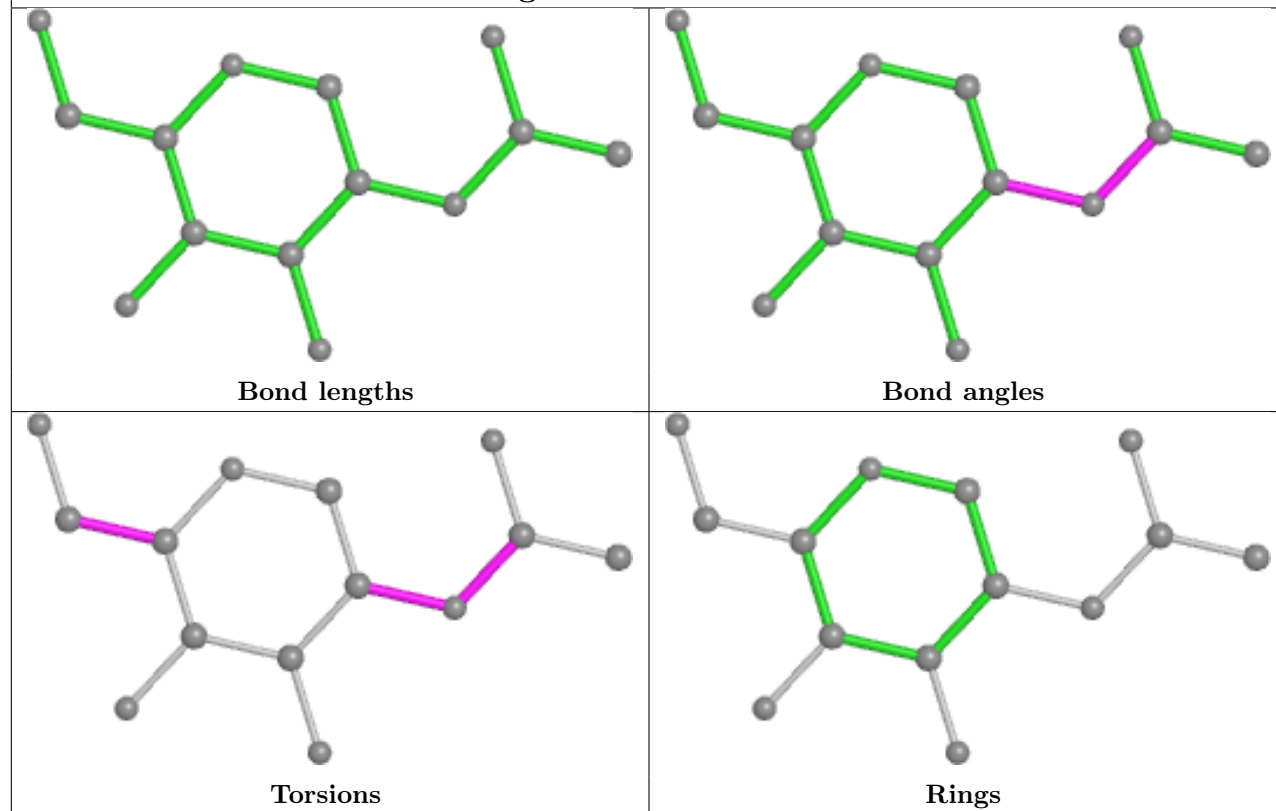
Ligand NAG B 1406



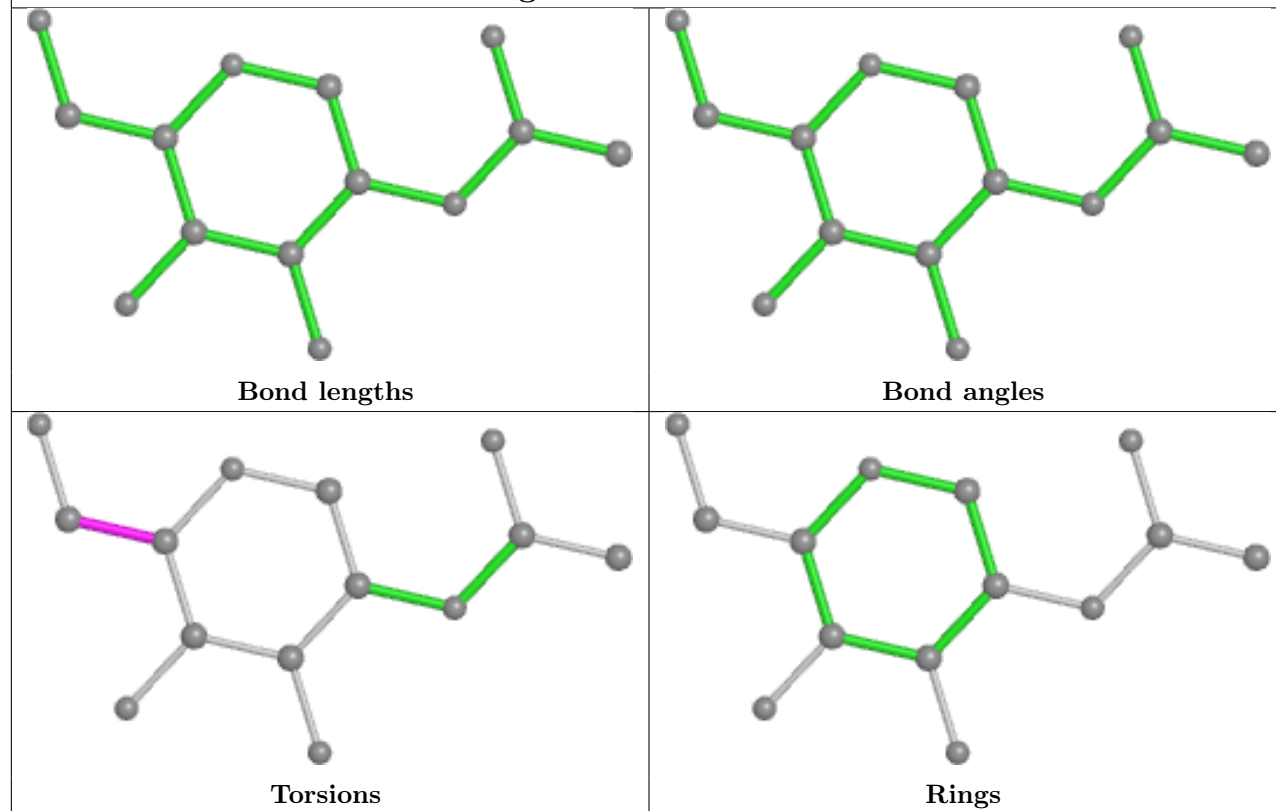
Ligand NAG C 1403



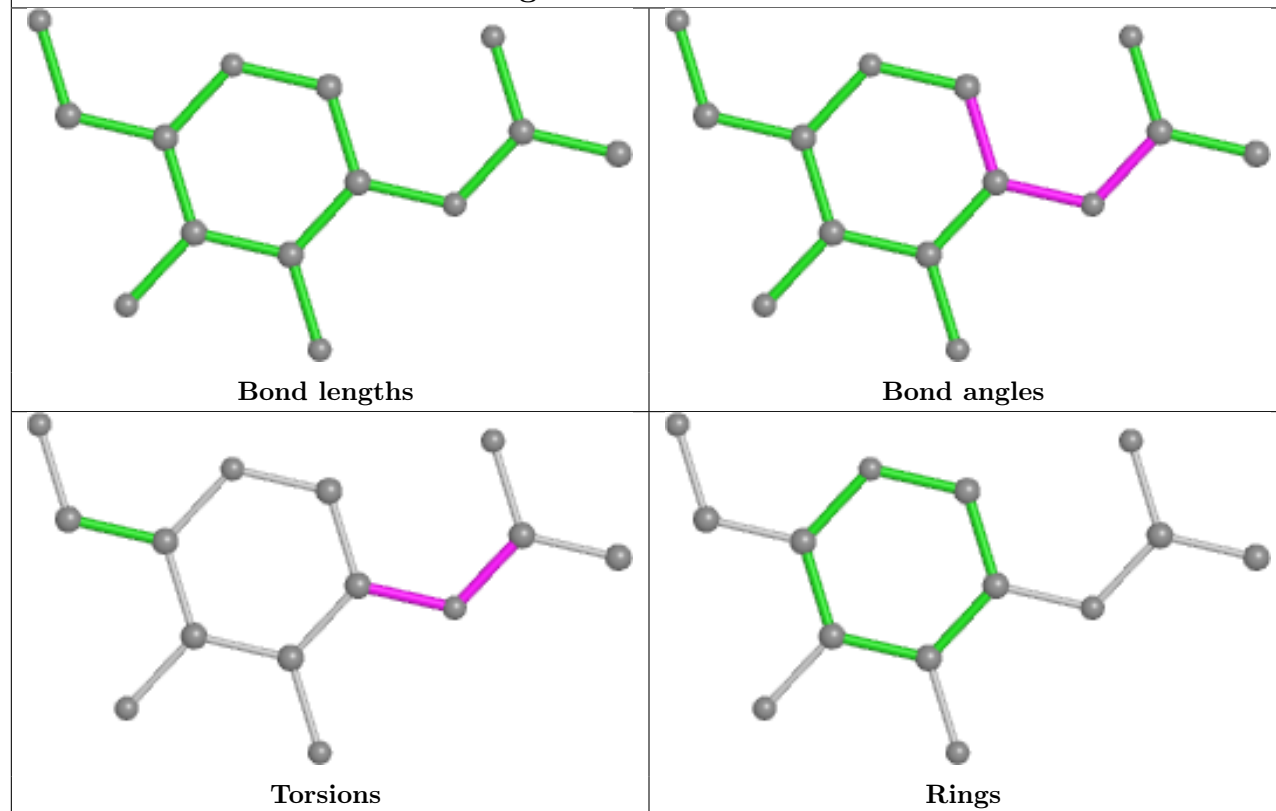
Ligand NAG A 1405



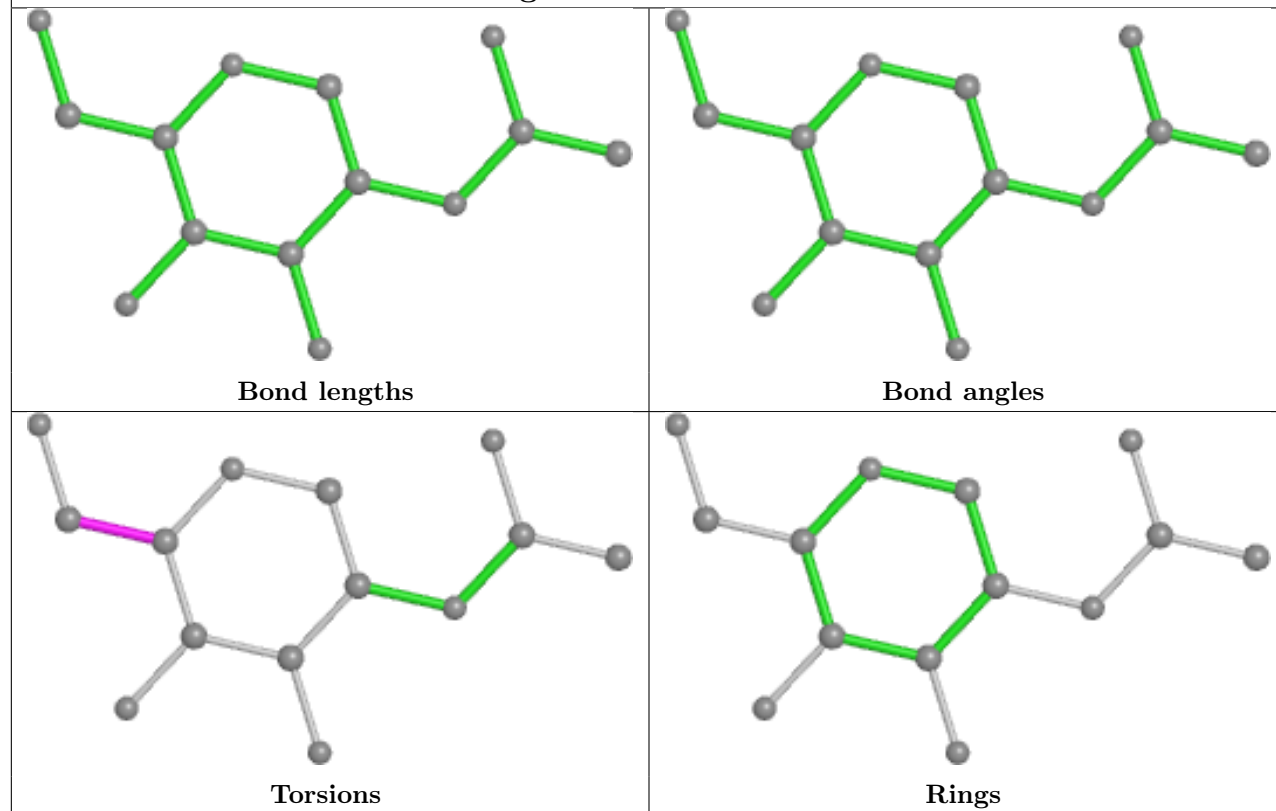
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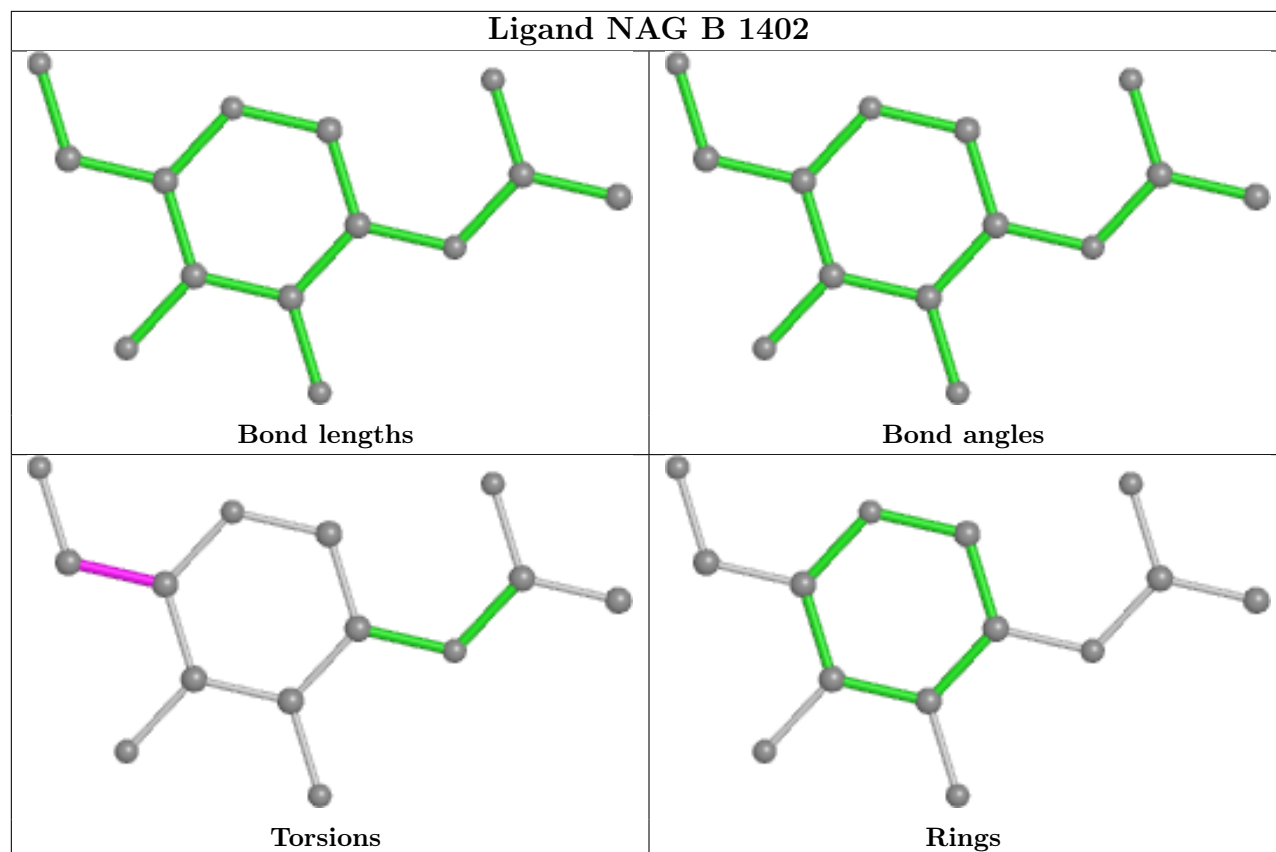
Ligand NAG C 1405



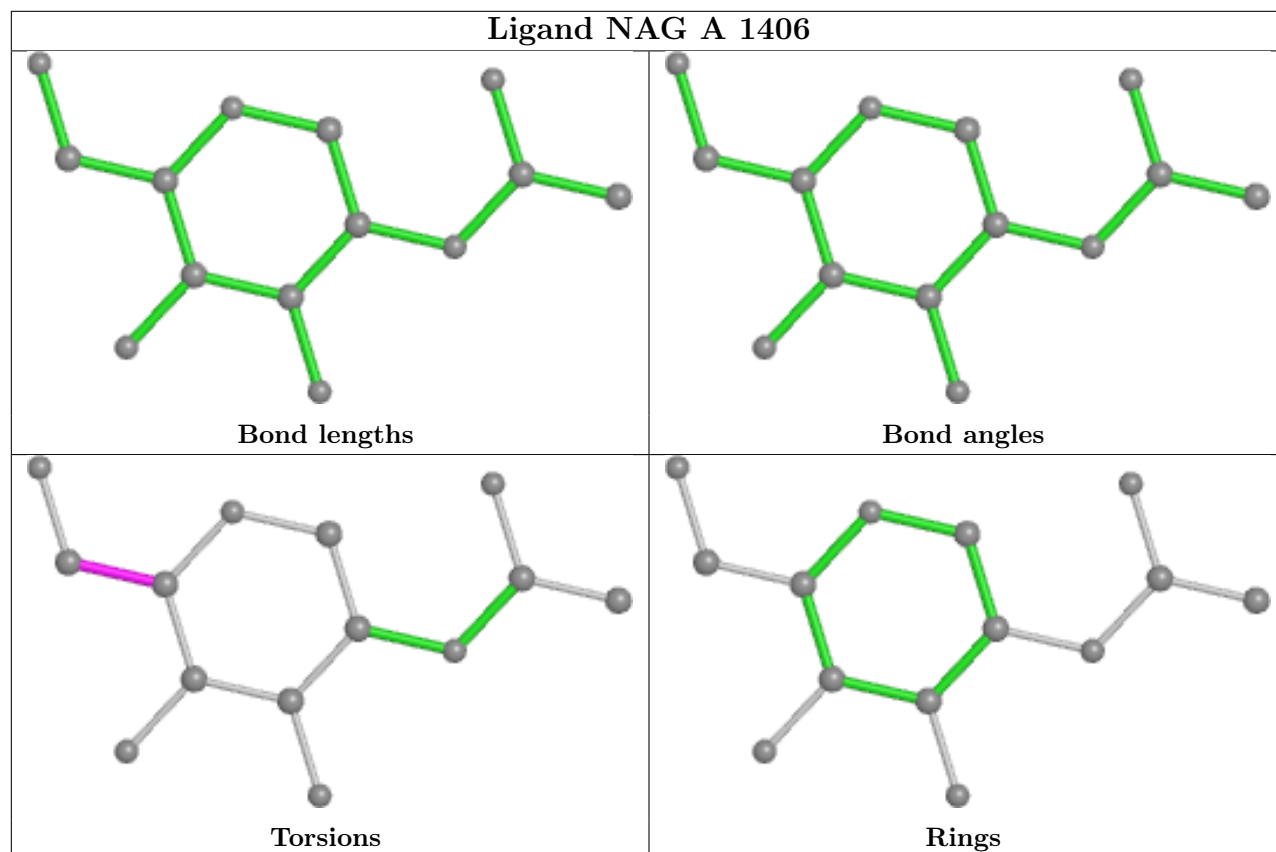
Ligand NAG B 1407

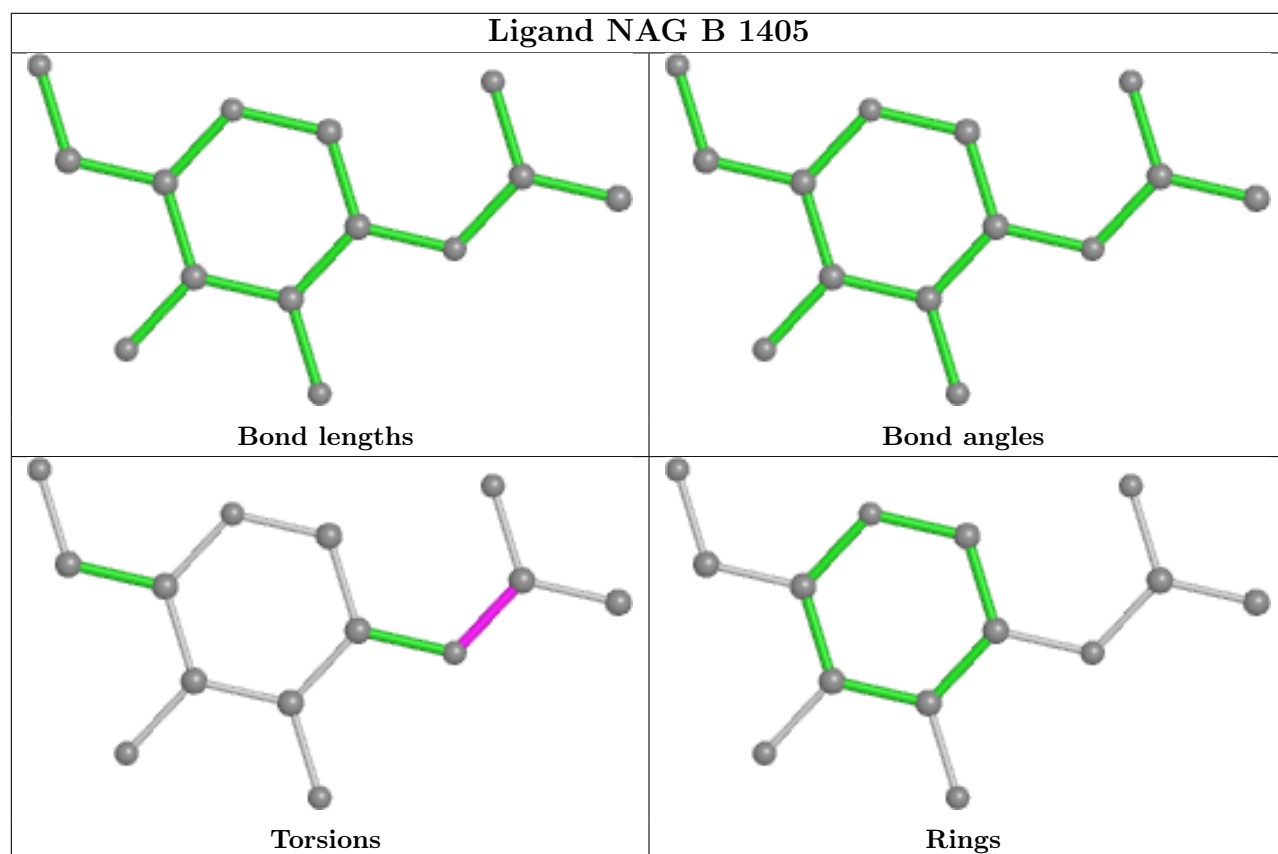
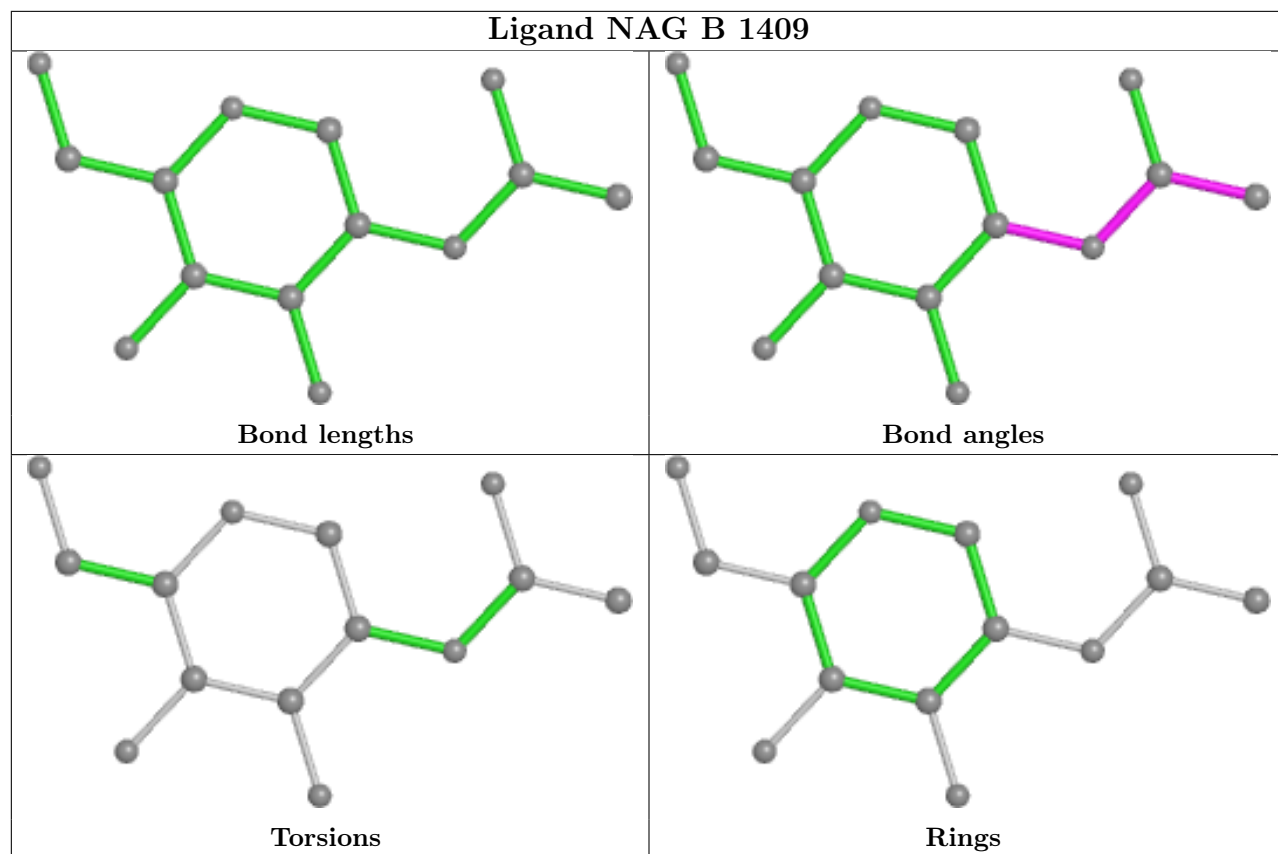


Ligand NAG B 1402

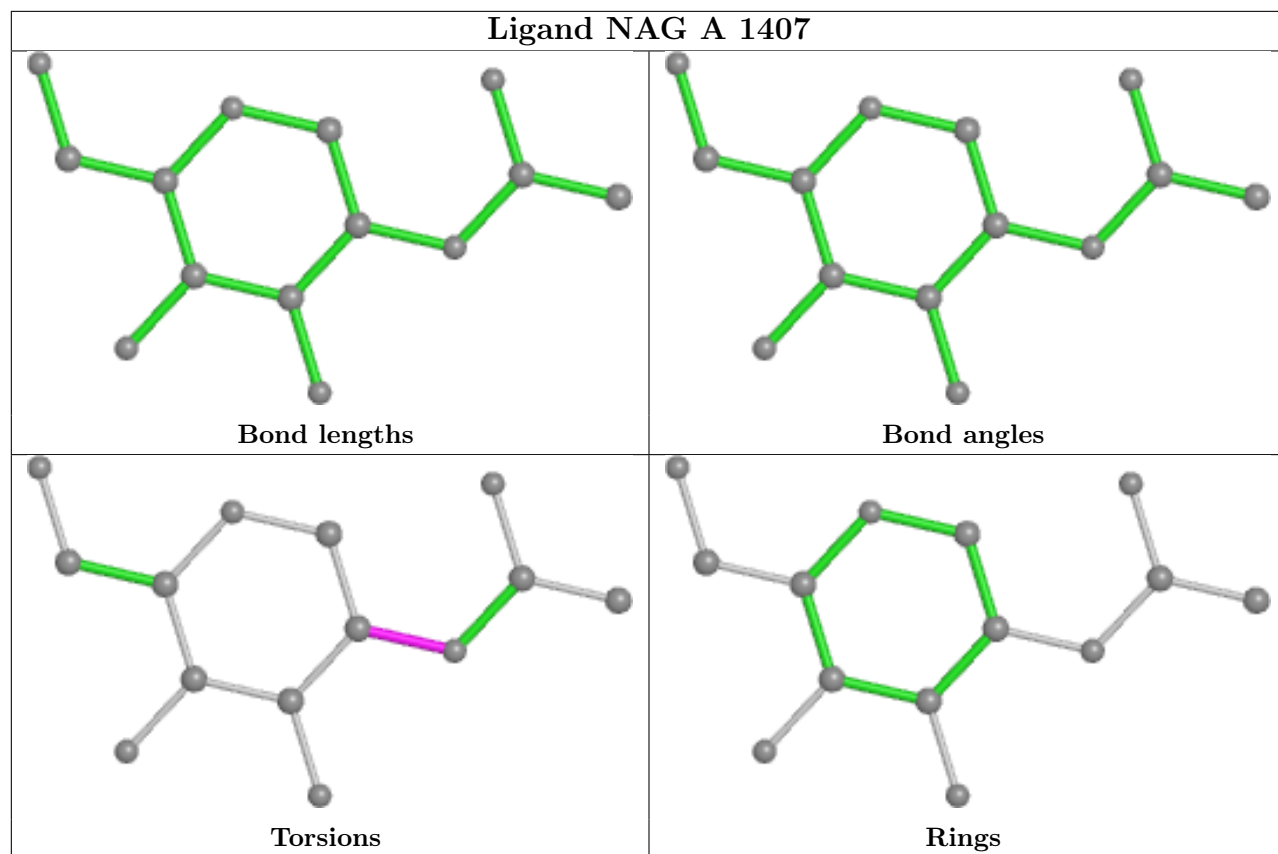


Ligand NAG A 1406

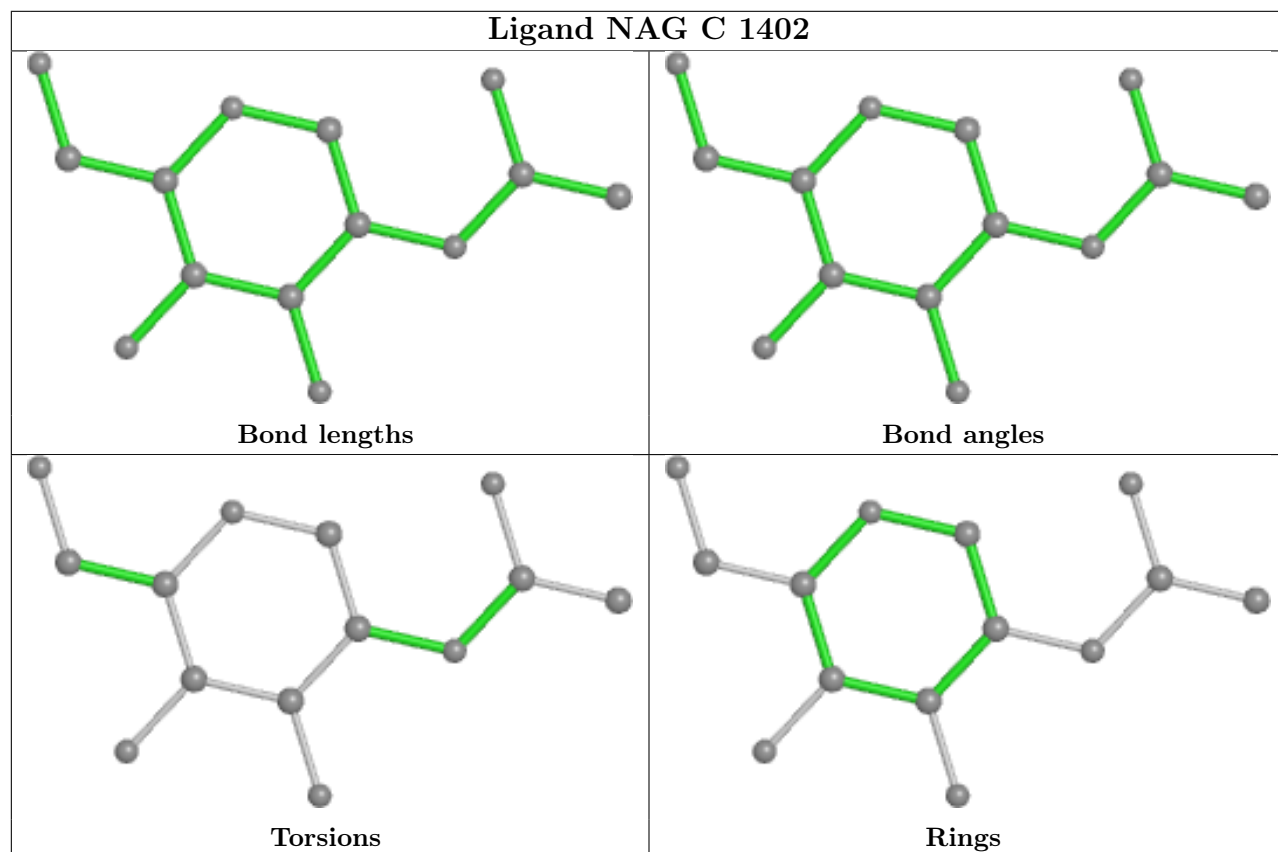


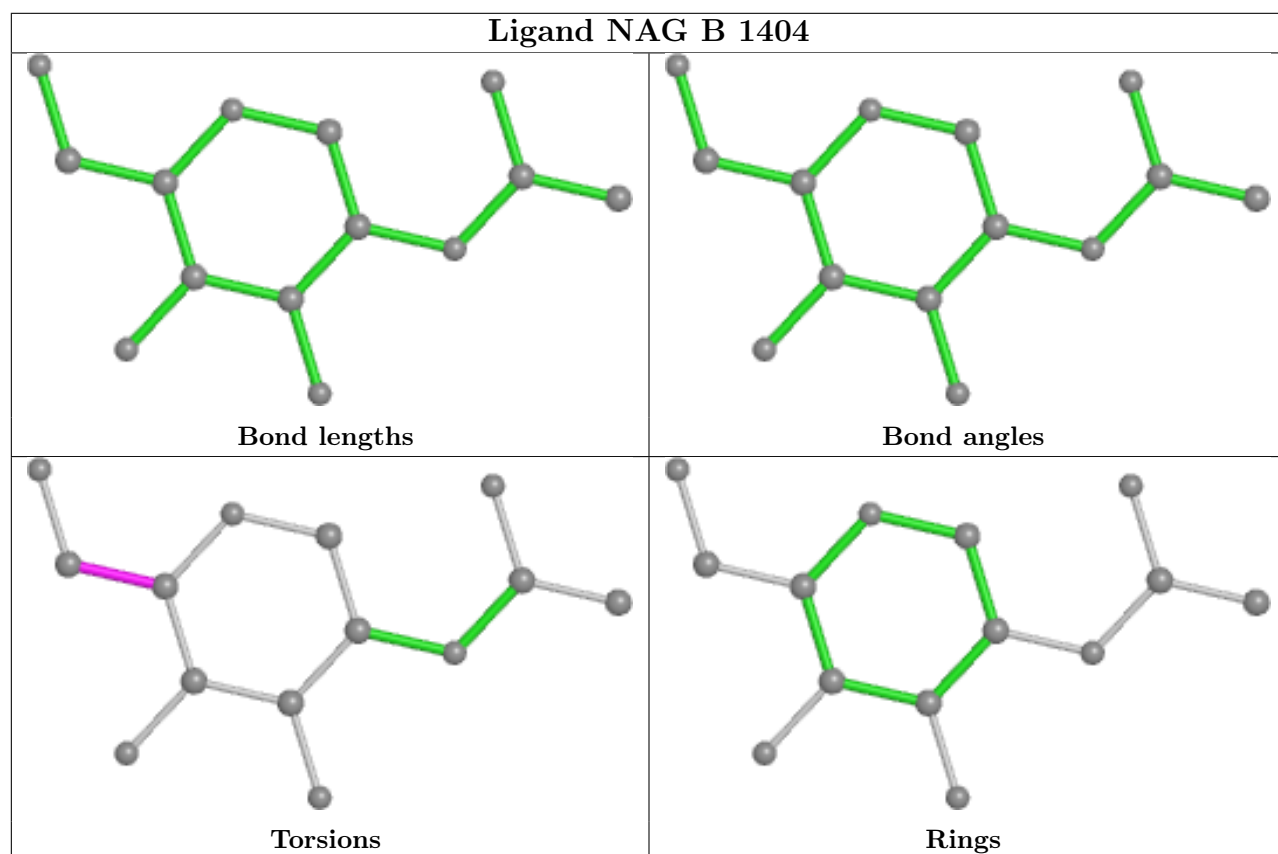
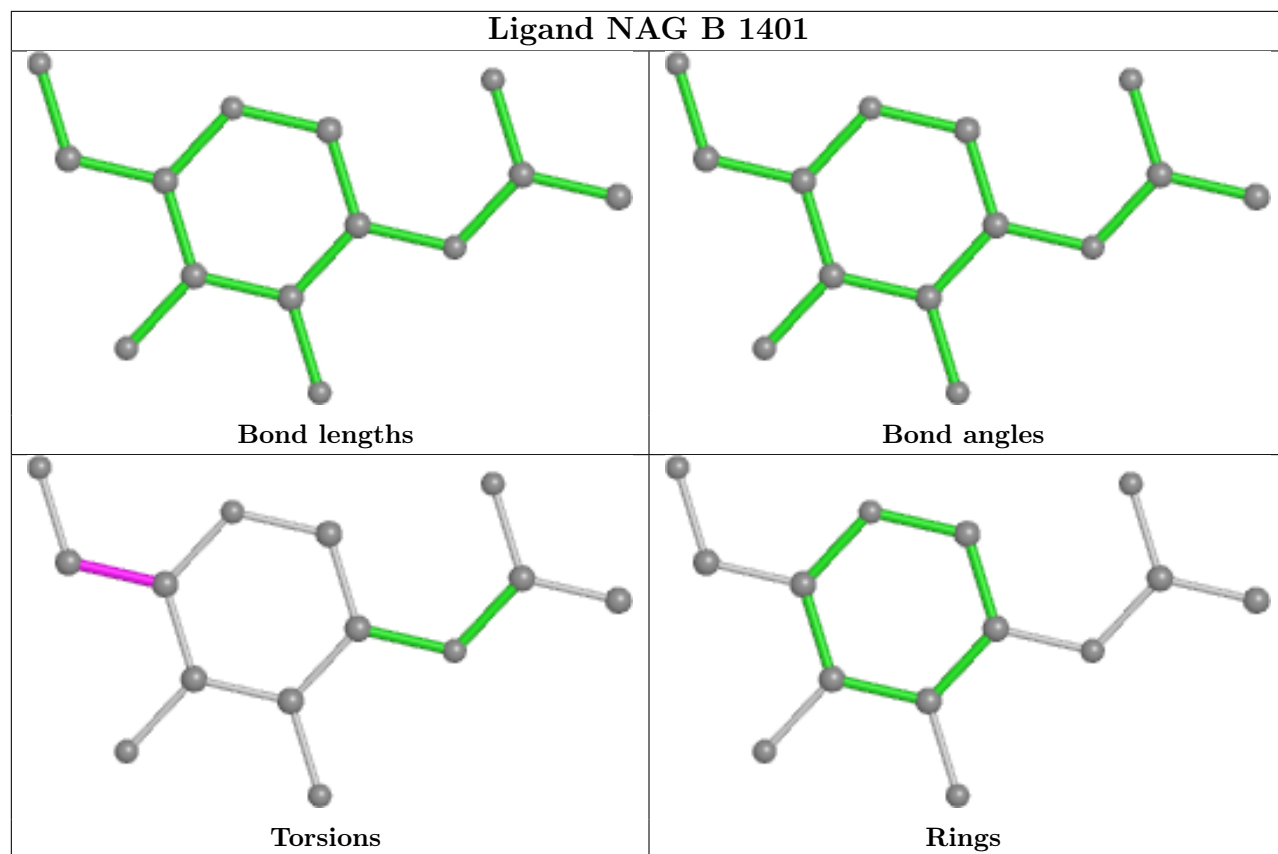


Ligand NAG A 1407

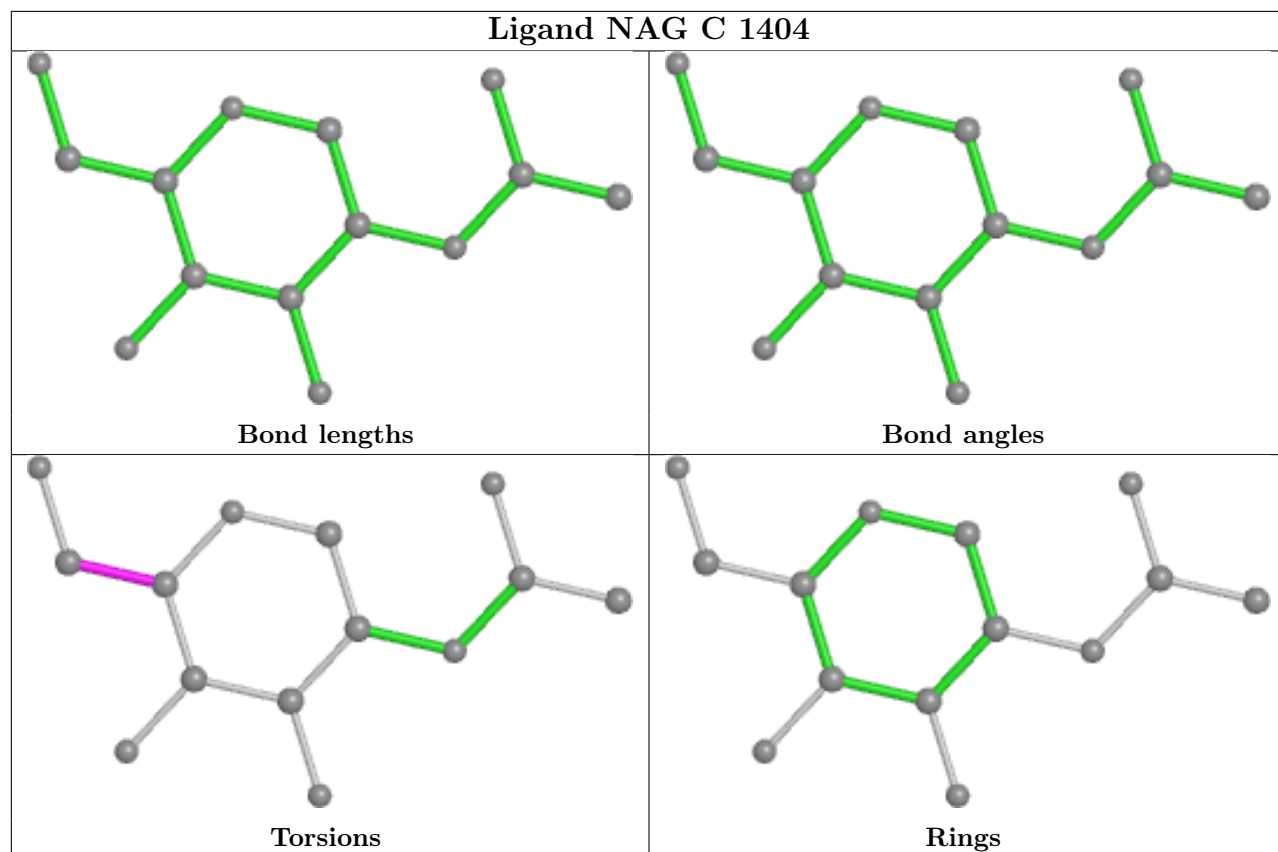


Ligand NAG C 1402

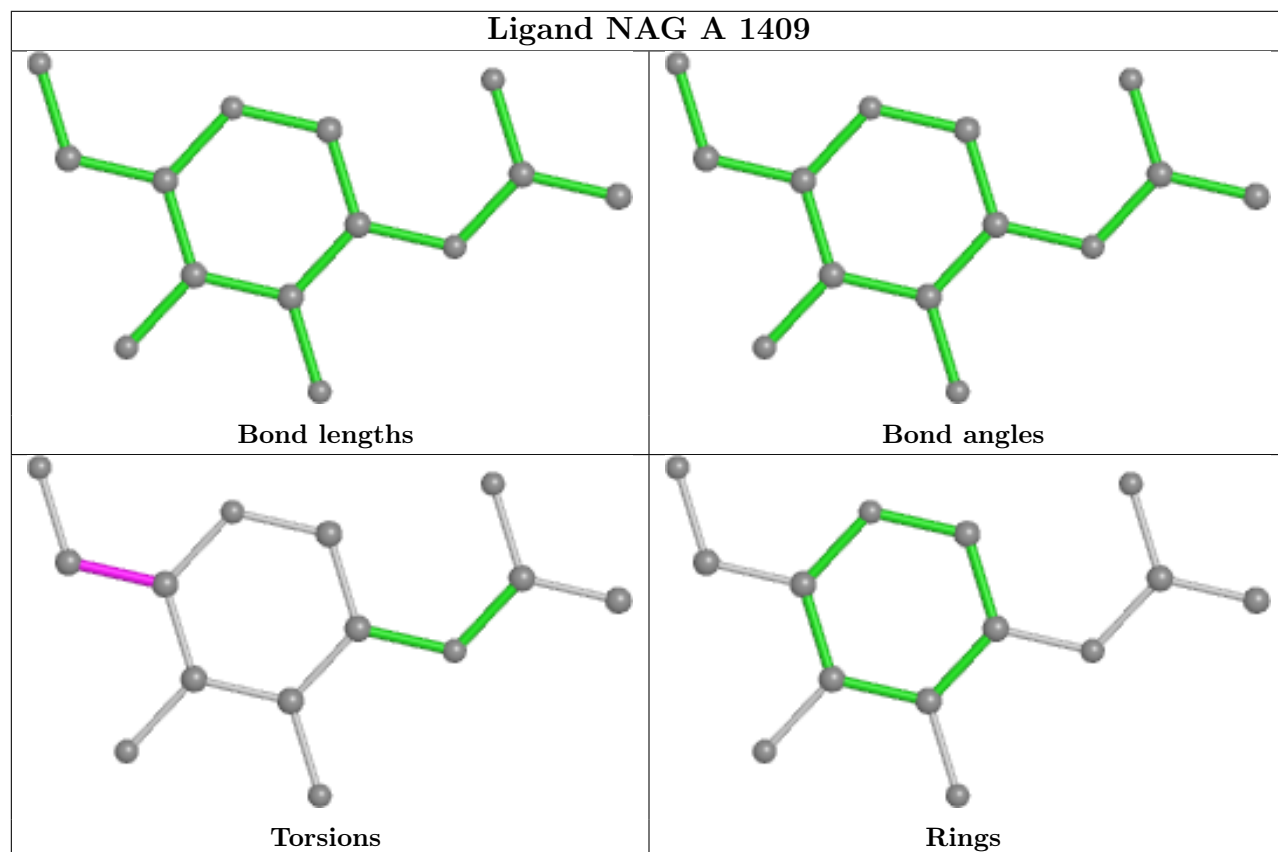




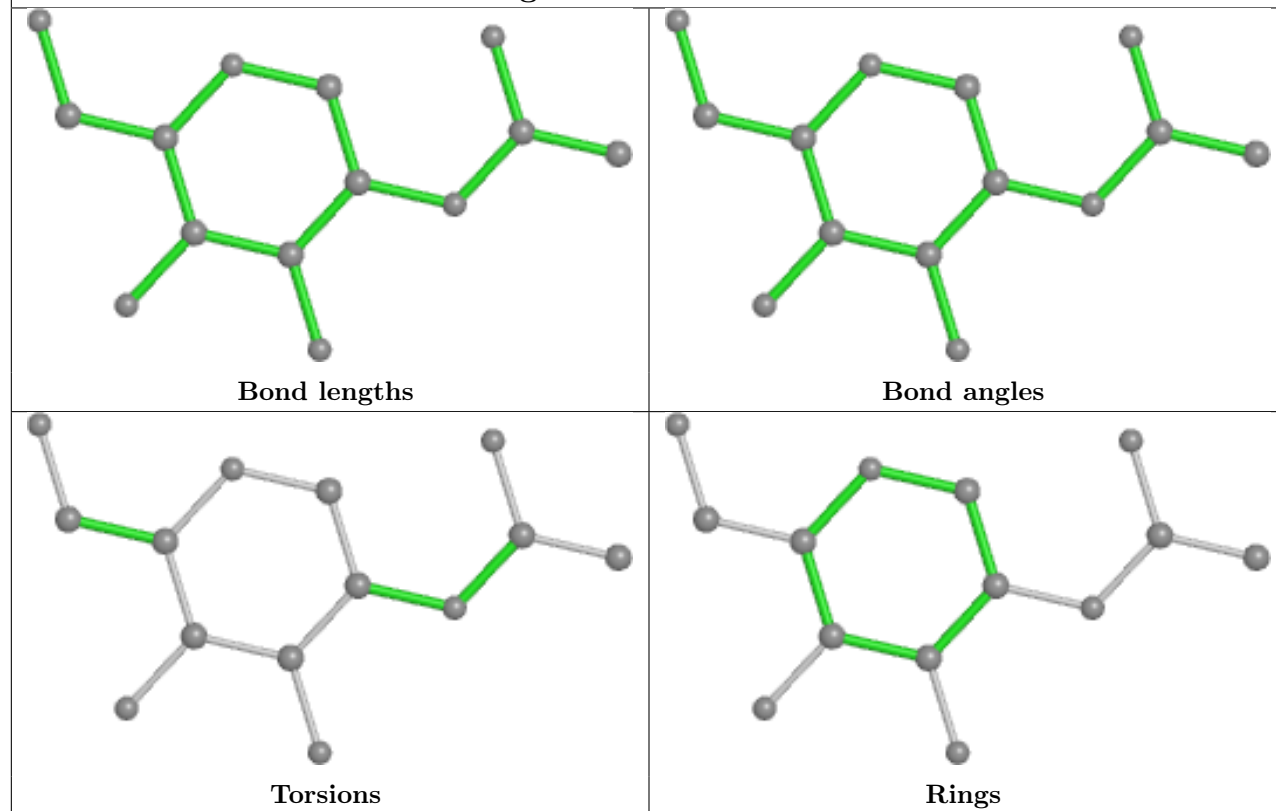
Ligand NAG C 1404



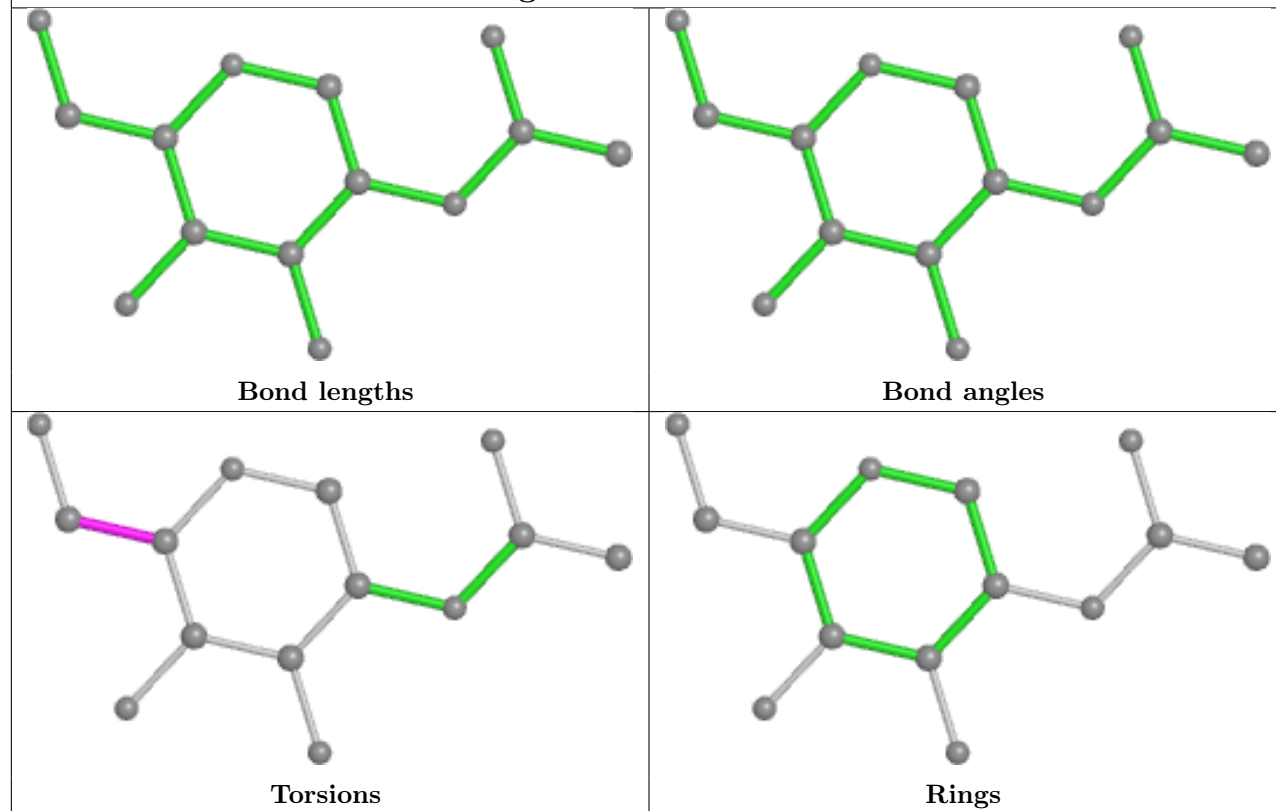
Ligand NAG A 1409



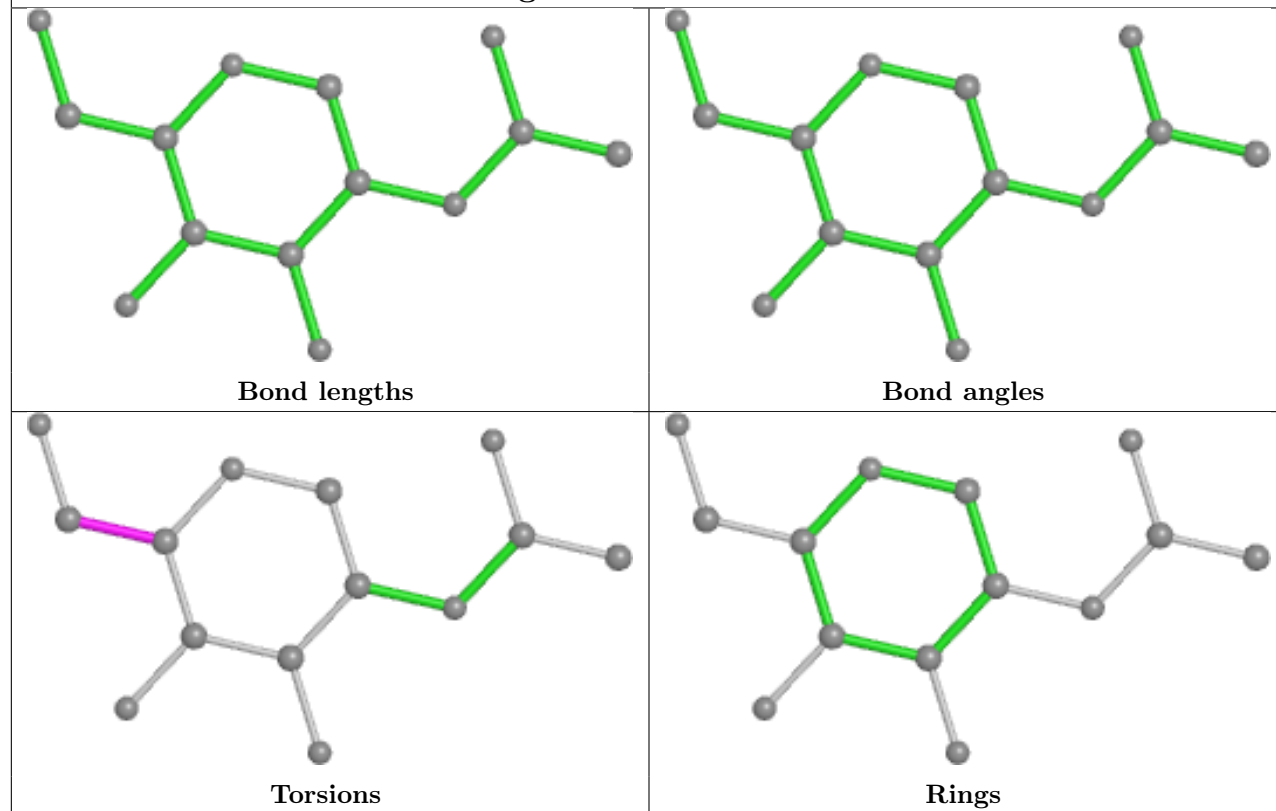
Ligand NAG B 1410



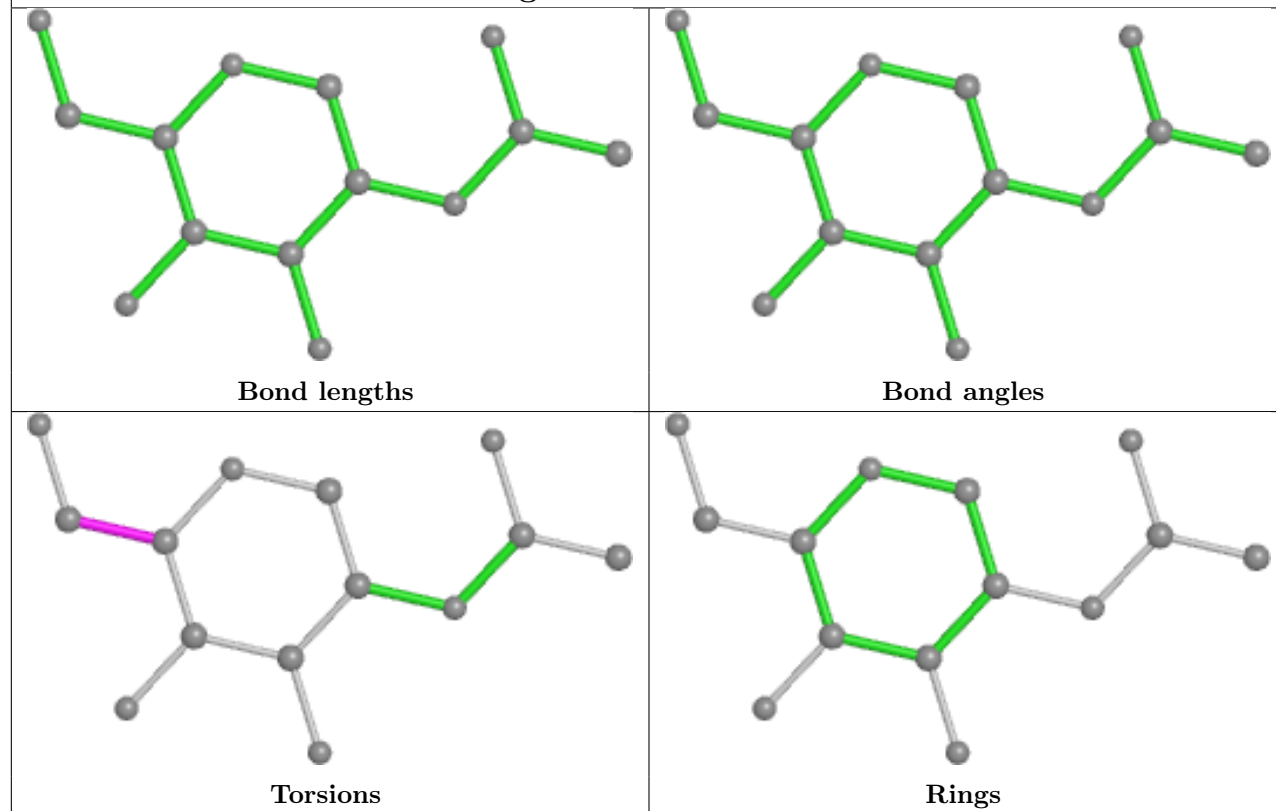
Ligand NAG A 1403



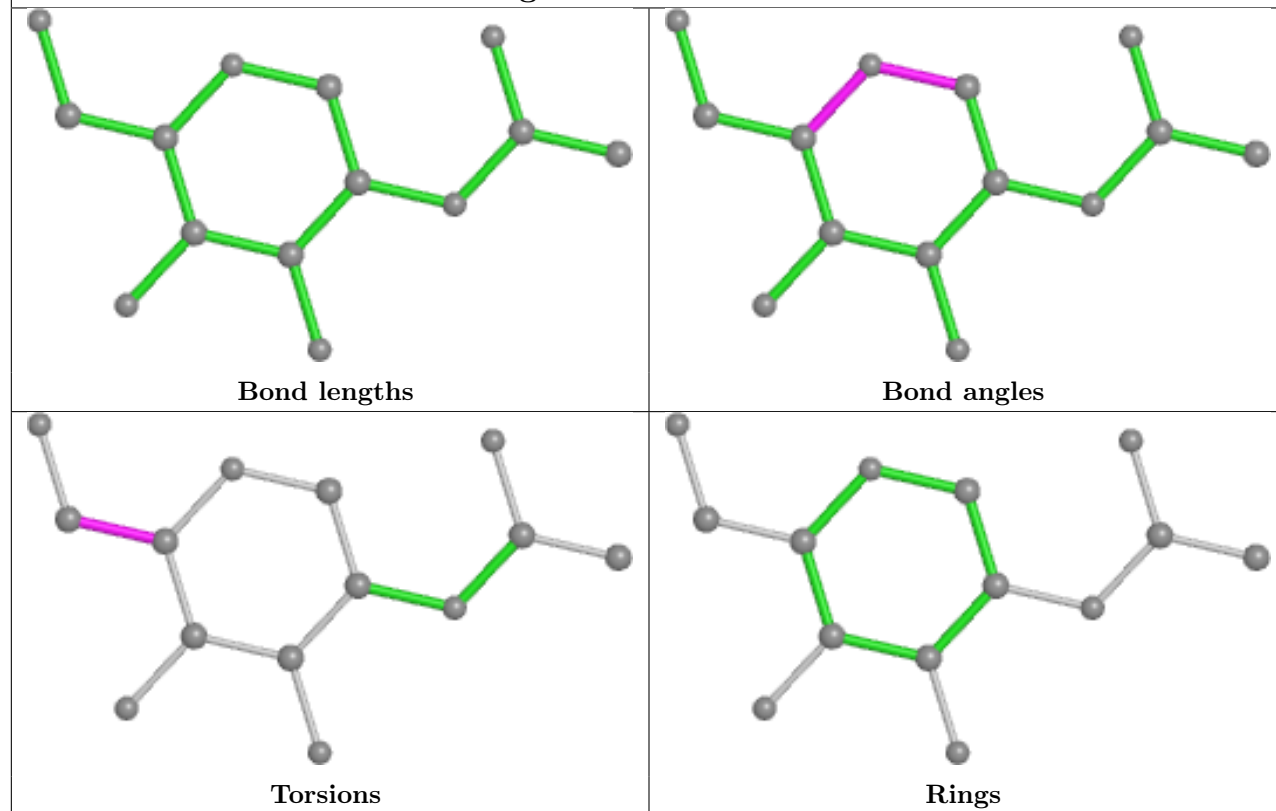
Ligand NAG A 1402



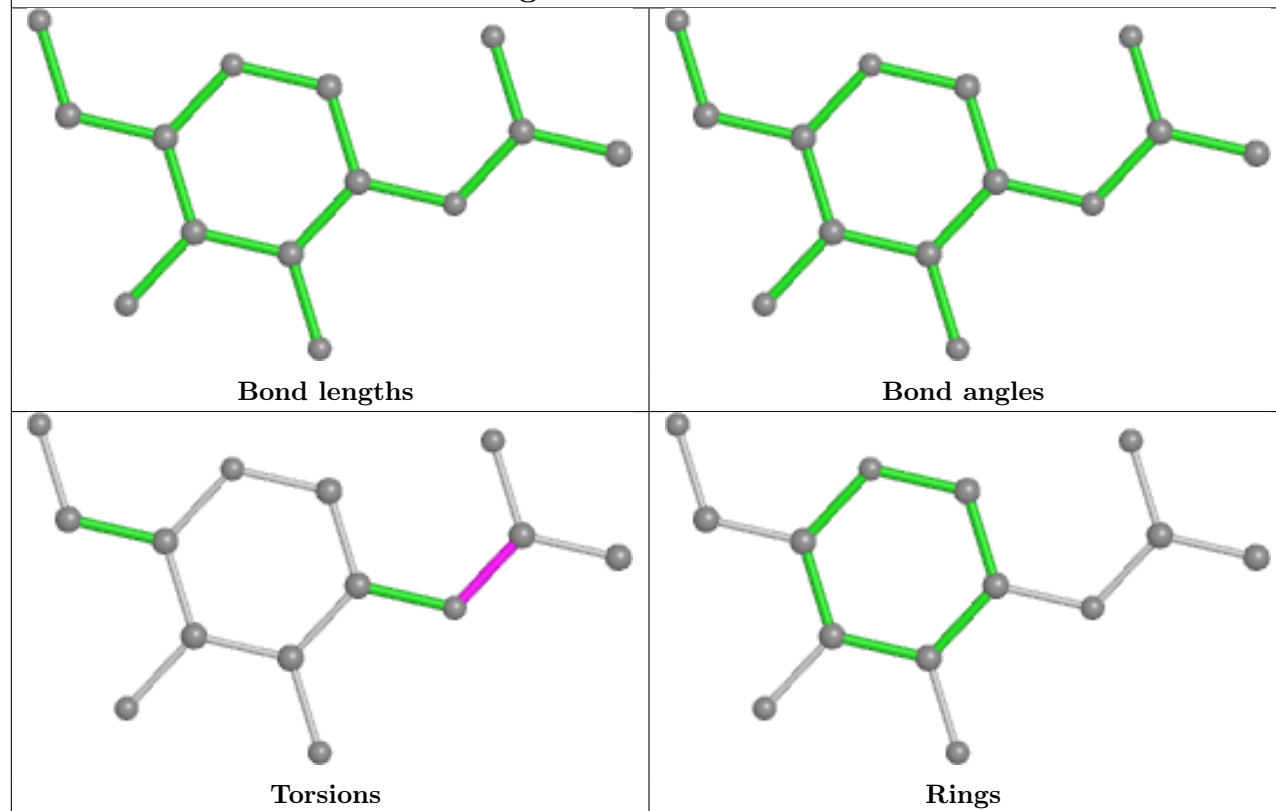
Ligand NAG C 1408



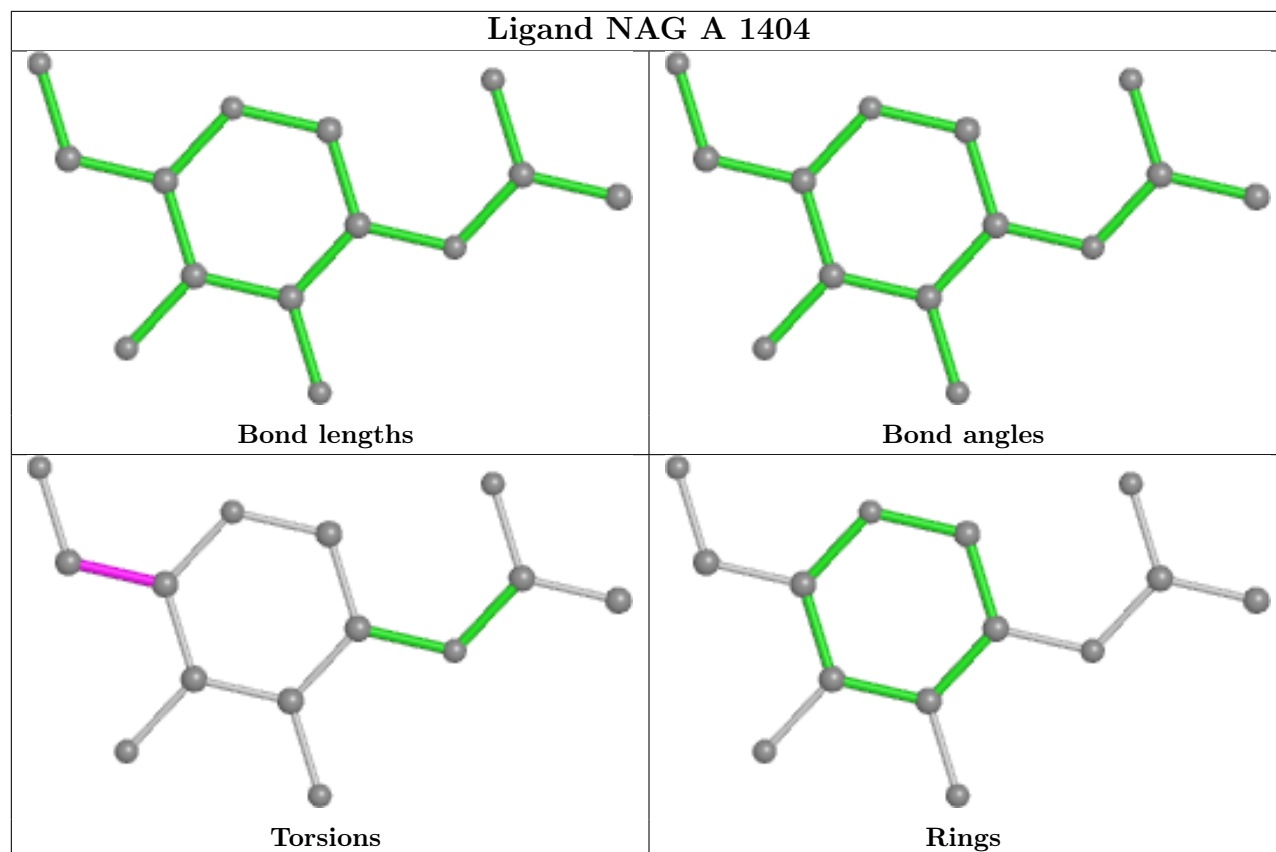
Ligand NAG C 1401



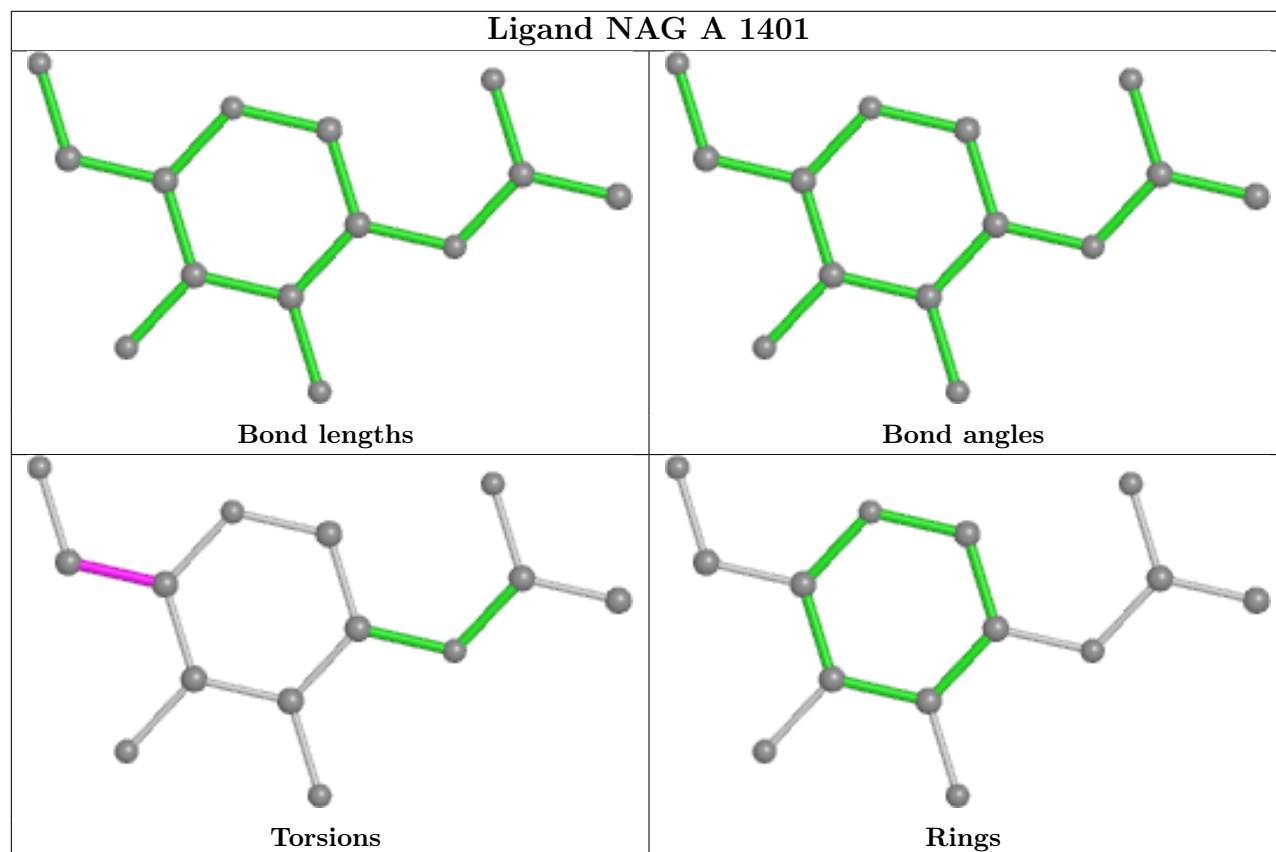
Ligand NAG C 1406

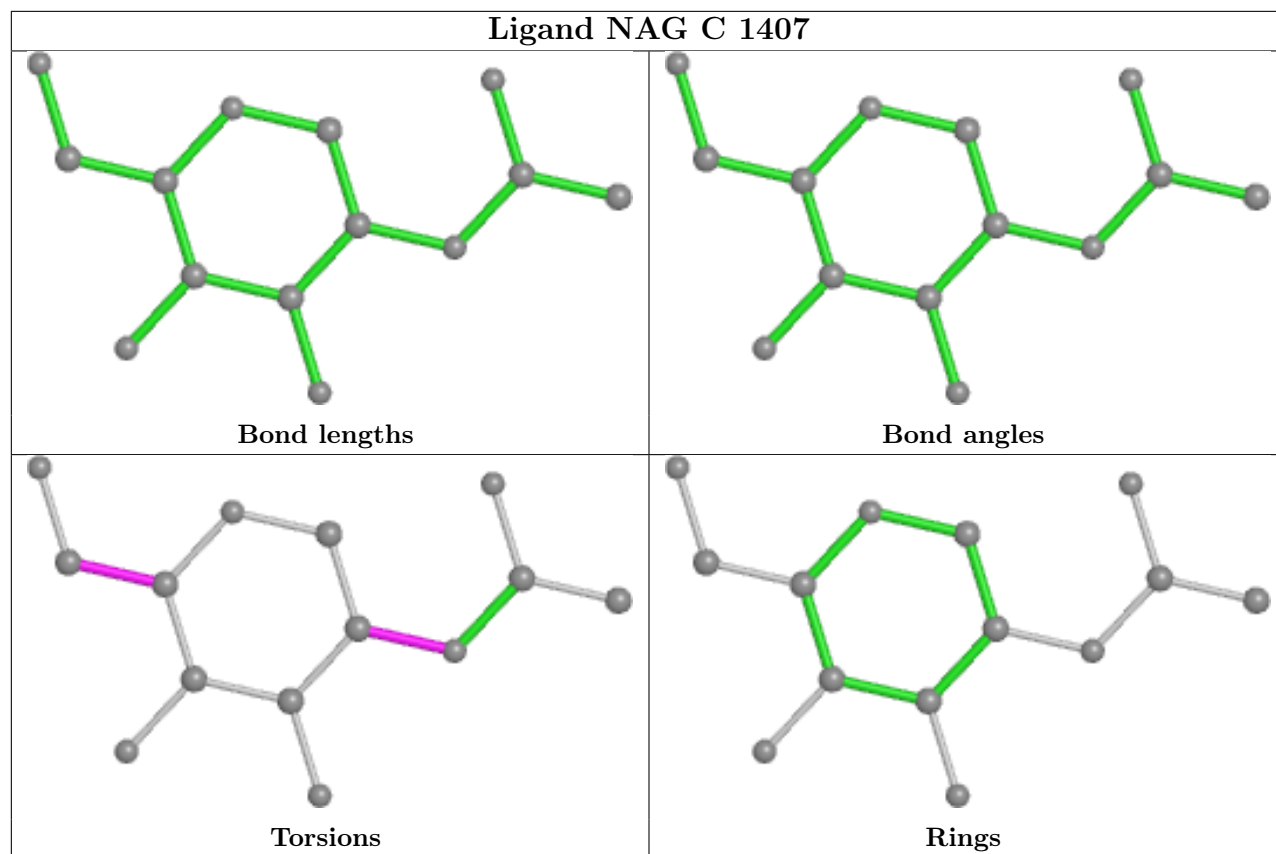


Ligand NAG A 1404



Ligand NAG A 1401





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.

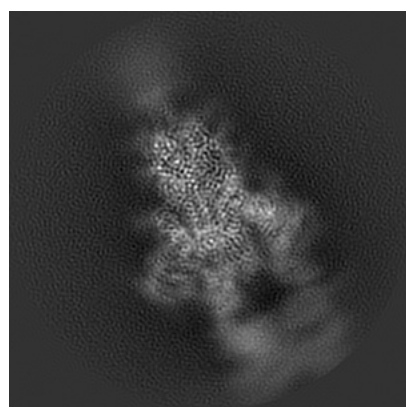
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30522. These allow visual inspection of the internal detail of the map and identification of artifacts.

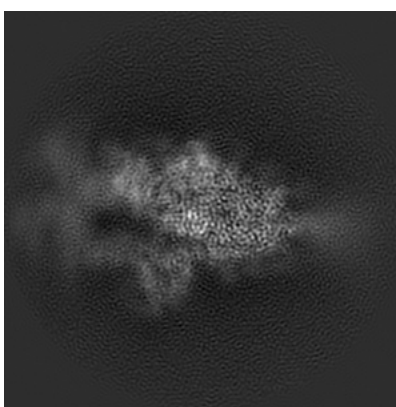
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

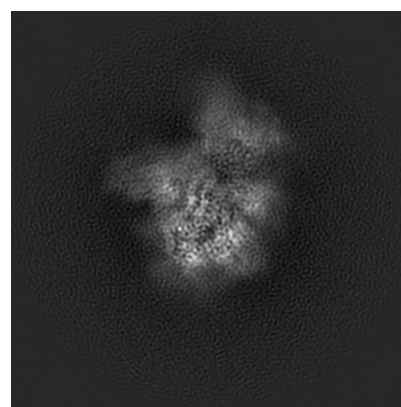
6.1.1 Primary map



X



Y

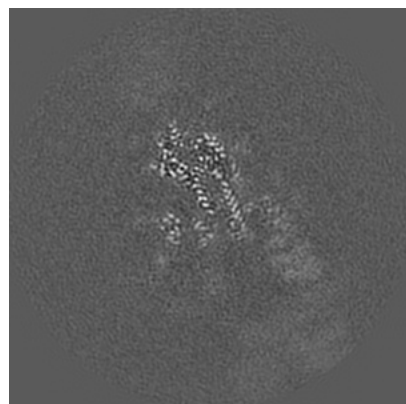


Z

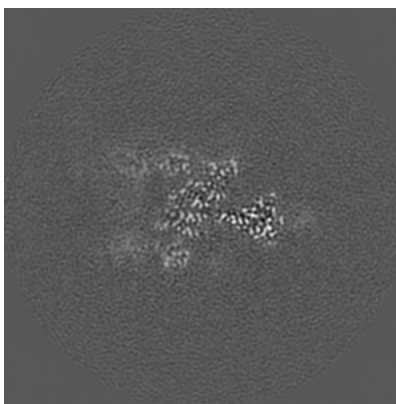
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

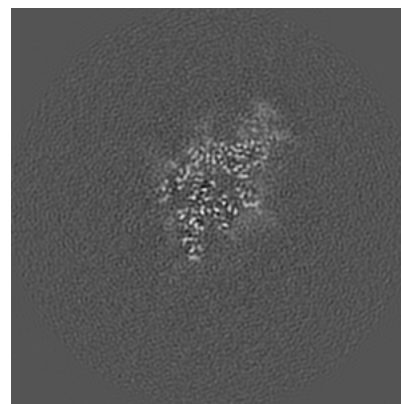
6.2.1 Primary map



X Index: 144



Y Index: 144

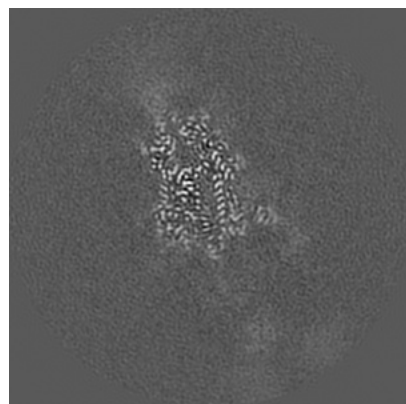


Z Index: 144

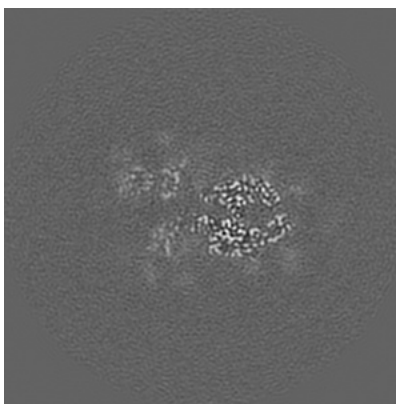
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

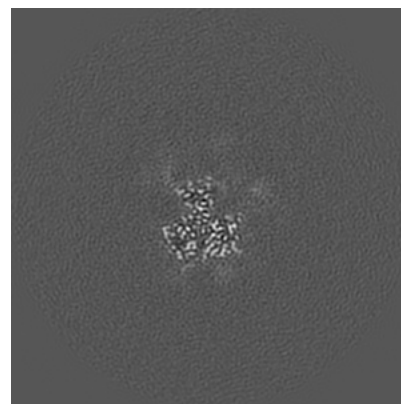
6.3.1 Primary map



X Index: 131



Y Index: 129

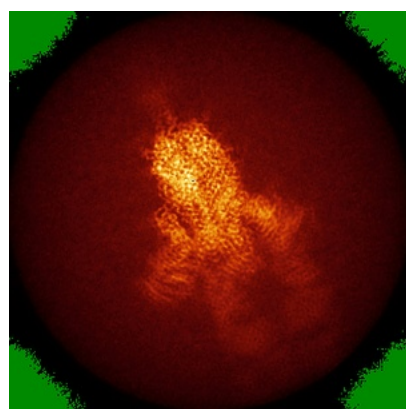


Z Index: 169

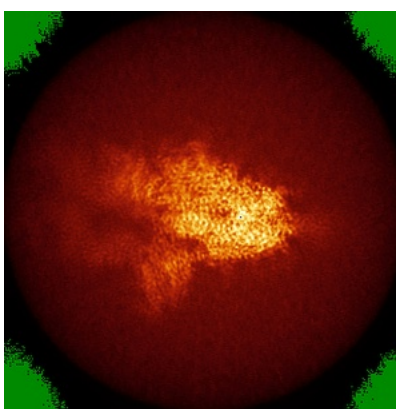
The images above show the largest variance slices of the map in three orthogonal directions.

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

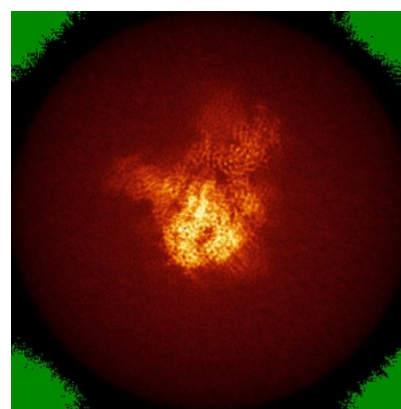
6.4.1 Primary map



X



Y



Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

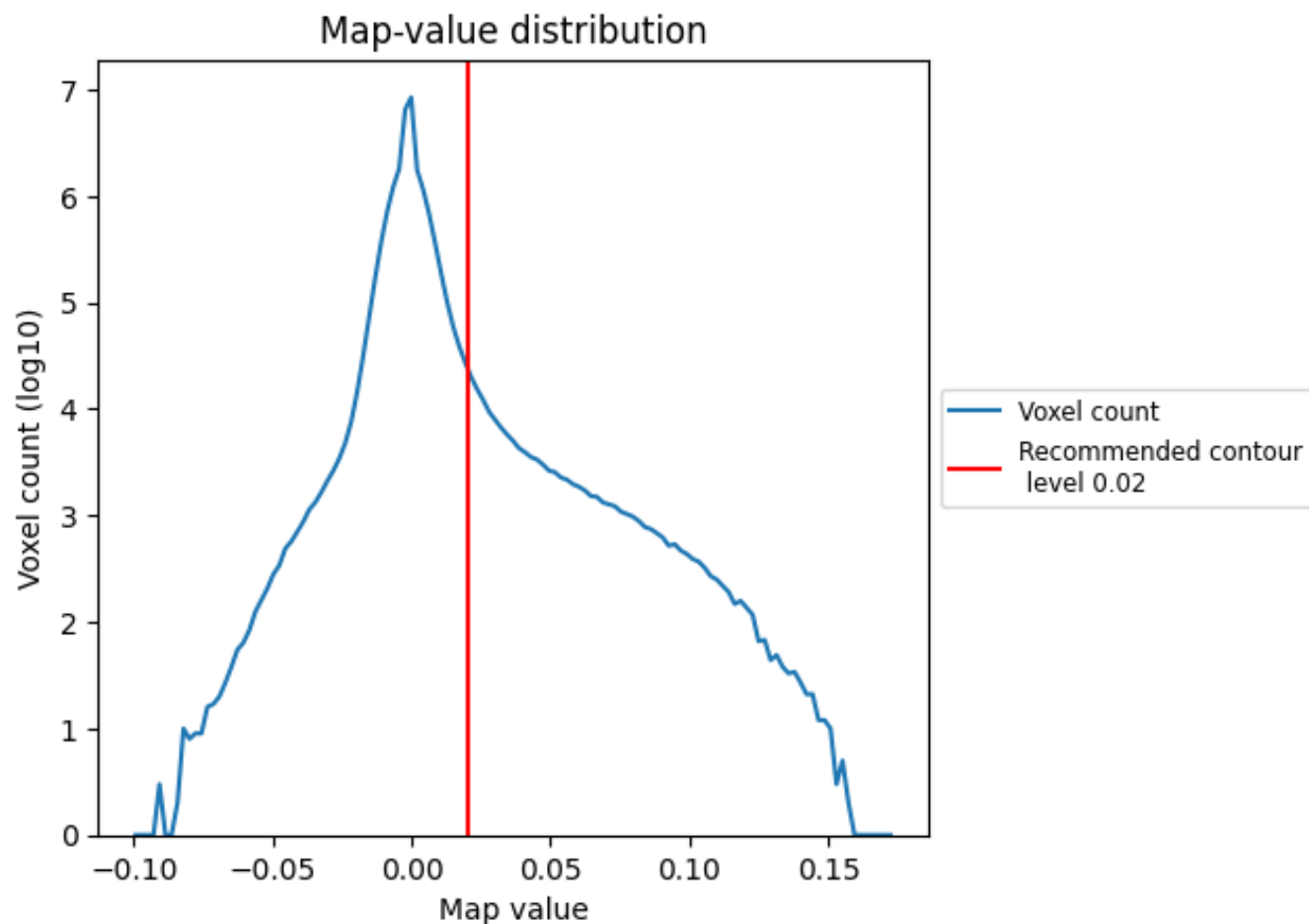
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

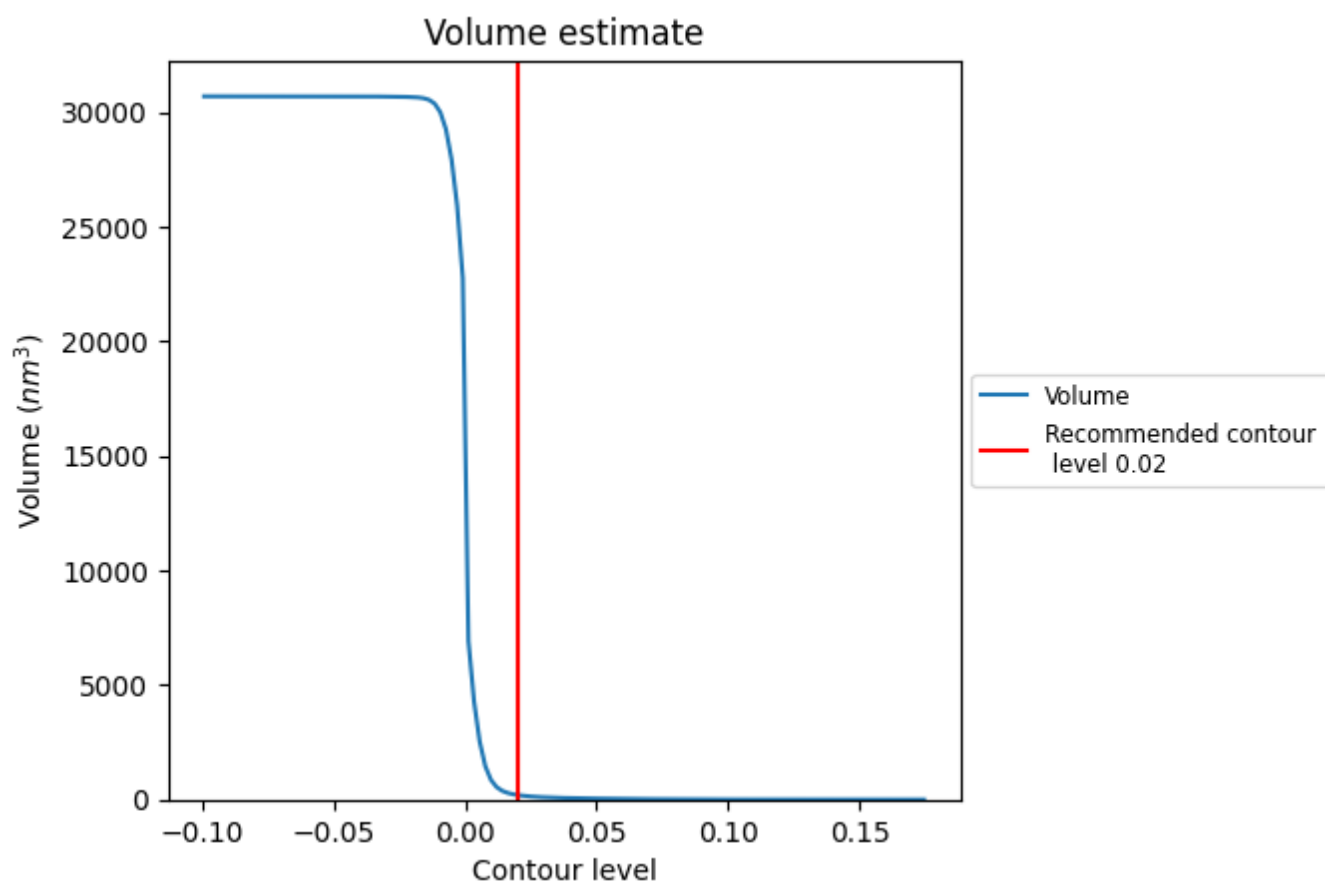
This section contains the results of statistical analysis of the map.

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.

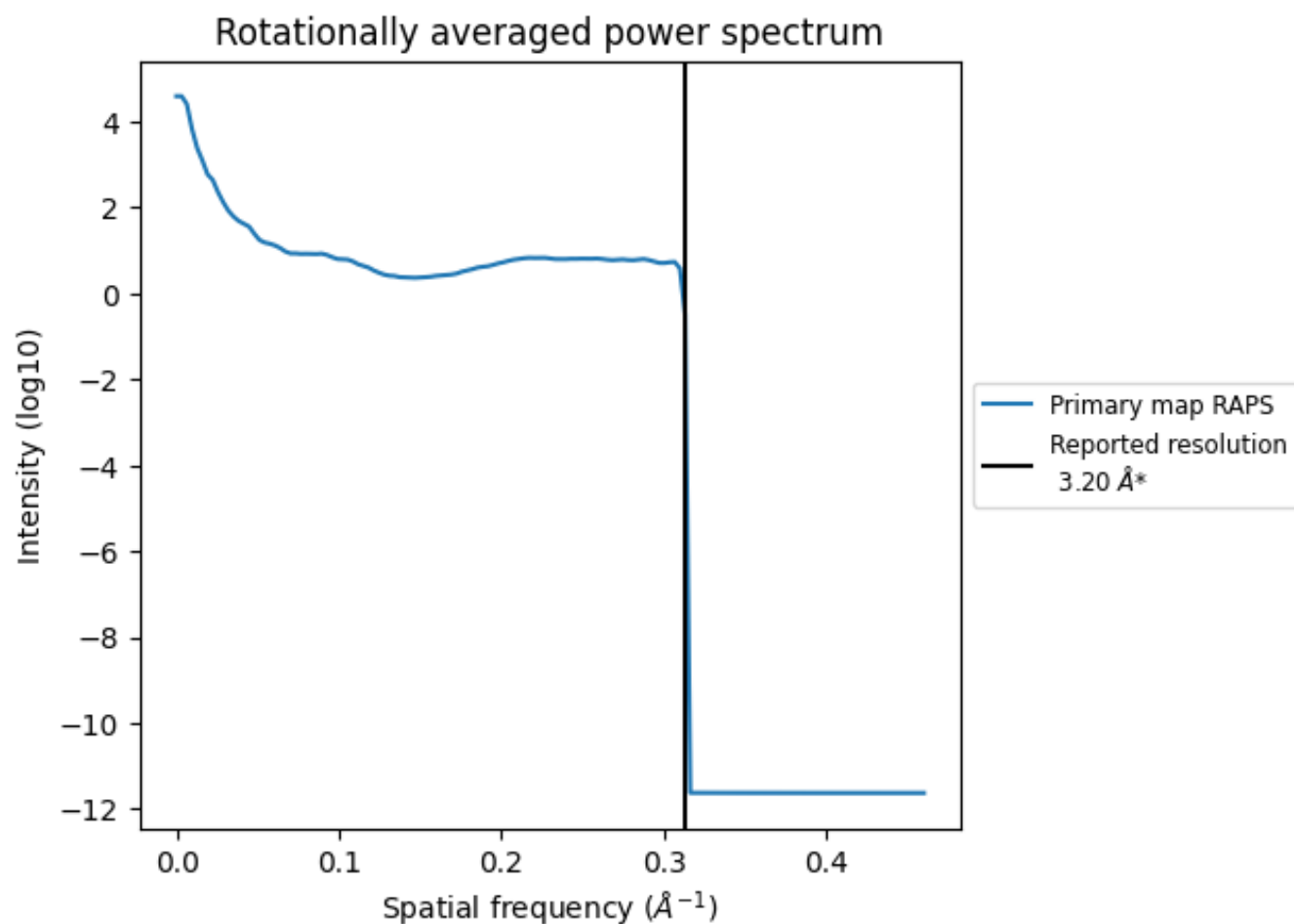
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196 nm³; this corresponds to an approximate mass of 177 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 0.312 Å⁻¹

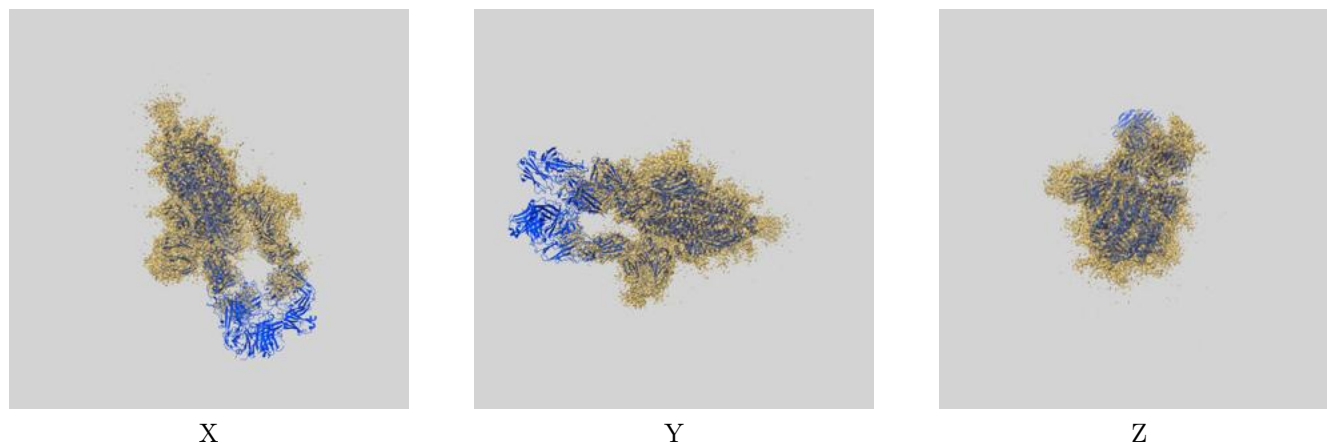
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

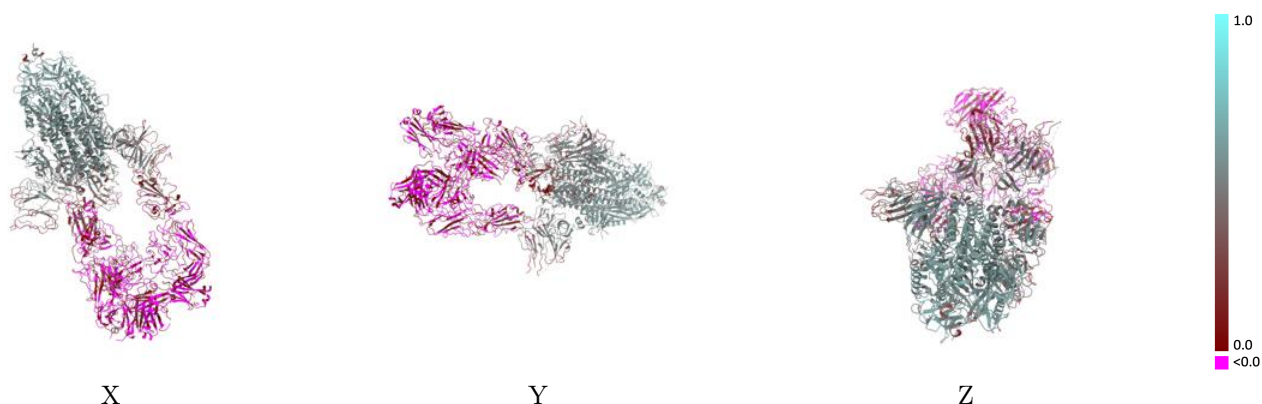
This section contains information regarding the fit between EMDB map EMD-30522 and PDB model 7CZZ. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



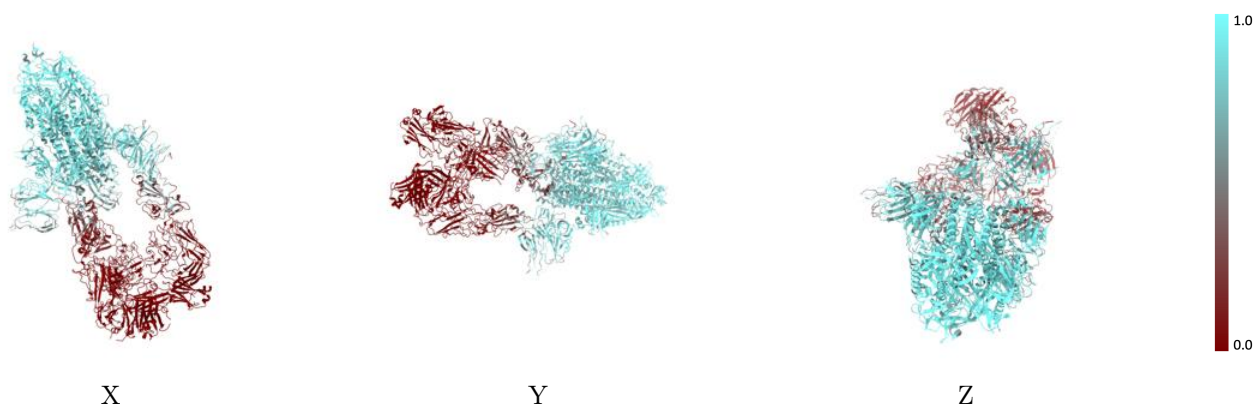
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



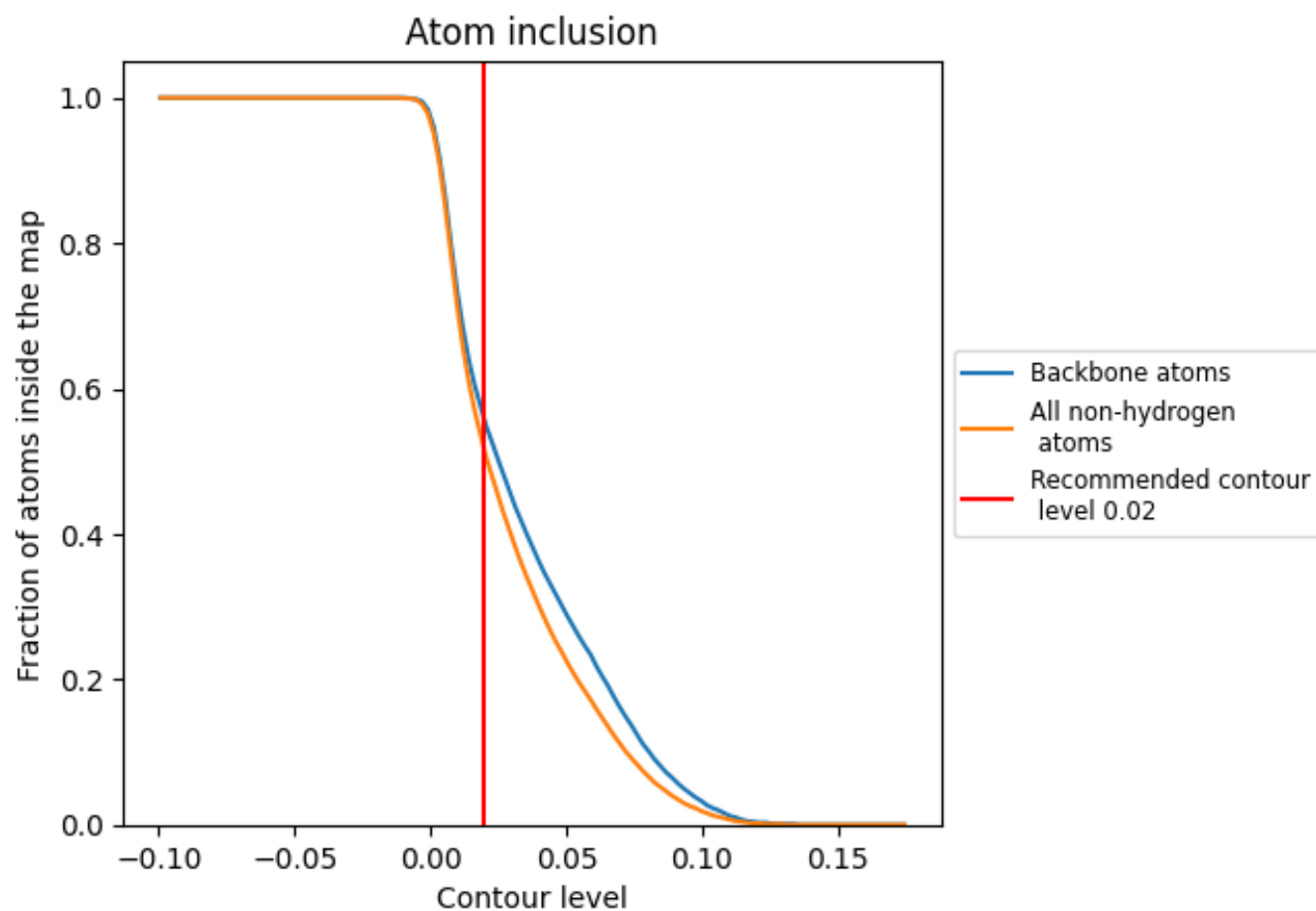
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 51% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5140	 0.2980
A	 0.7430	 0.4250
B	 0.7190	 0.4140
C	 0.7120	 0.4100
D	 0.6430	 0.3110
E	 0.1790	 -0.0190
F	 0.9290	 0.5400
G	 0.6790	 0.4140
H	 0.0330	 0.0050
I	 0.0060	 0.0290
J	 0.0050	 0.0110
K	 0.0190	 0.0170
L	 0.6430	 0.4500
M	 0.0020	 0.0250
N	 0.0070	 0.0120
O	 0.8570	 0.4810
P	 0.7140	 0.4180
Q	 0.4640	 0.0560
R	 0.0360	 0.0810
S	 0.5000	 0.3050
T	 0.8210	 0.4580
U	 0.7140	 0.3550
V	 0.8210	 0.4550
W	 0.7140	 0.4210
X	 0.4640	 0.1860
Y	 0.1070	 0.1330
Z	 0.4640	 0.2380
a	 0.7860	 0.5020
b	 0.6070	 0.2540
c	 0.5360	 0.3130
d	 0.8570	 0.4710
e	 0.7140	 0.3100
f	 0.0240	 0.1740
g	 0.0240	 0.0230
h	 0.0000	 0.0210

