



## wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 12:42 PM JST

PDB ID : 7D0D  
EMDB ID : EMD-30531  
Title : S protein of SARS-CoV-2 in complex bound with P5A-3C12\_2B  
Authors : Yan, R.H.; Wang, R.K.; Ju, B.; Yu, J.F.; Zhang, Y.Y.; Liu, N.; Wang, H.W.;  
Wang, X.Q.; Zhang, L.Q.; Zhou, Q.  
Deposited on : 2020-09-09  
Resolution : 3.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

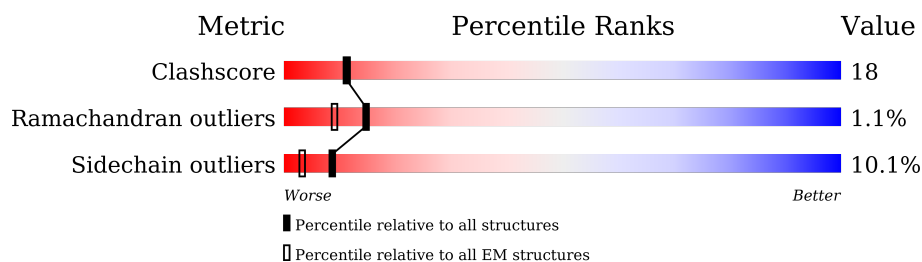
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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.



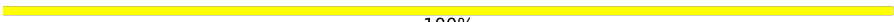







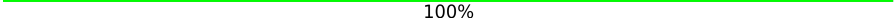



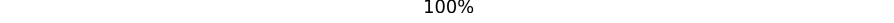
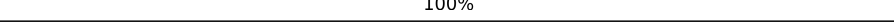







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	
1	B	1283	
1	C	1283	
2	G	226	
2	H	226	
3	F	220	
3	L	220	
4	D	2	

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Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	I	2	 50% 50%
4	J	2	 50% 50%
4	K	2	 100%
4	M	2	 50% 50%
4	N	2	 100%
4	O	2	 100%
4	P	2	 50% 50%
4	Q	2	 100%
4	R	2	 50% 50%
4	S	2	 50% 50%
4	T	2	 50% 50%
4	U	2	 100%
4	V	2	 100%
4	W	2	 50% 50%
4	X	2	 50% 50%
4	Y	2	 50% 50%
4	Z	2	 50% 50%
4	a	2	 50% 50%
4	b	2	 50% 50%
4	c	2	 50% 50%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28096 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	1004	Total	C	N	O	S	0	0
			7853	5014	1307	1496	36		
1	C	982	Total	C	N	O	S	0	0
			7696	4920	1279	1462	35		
1	B	1006	Total	C	N	O	S	0	0
			7863	5019	1308	1500	36		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	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
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	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

- Molecule 2 is a protein called Heavy chain of P5A-3C12.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	125	Total	C	N	O	S	0	0
			972	625	154	189	4		
2	G	125	Total	C	N	O	S	0	0
			972	625	154	189	4		

- Molecule 3 is a protein called Light chain of P5A-3C12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	113	Total	C	N	O	S	0	0
			880	555	145	177	3		
3	F	113	Total	C	N	O	S	0	0
			880	555	145	177	3		

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



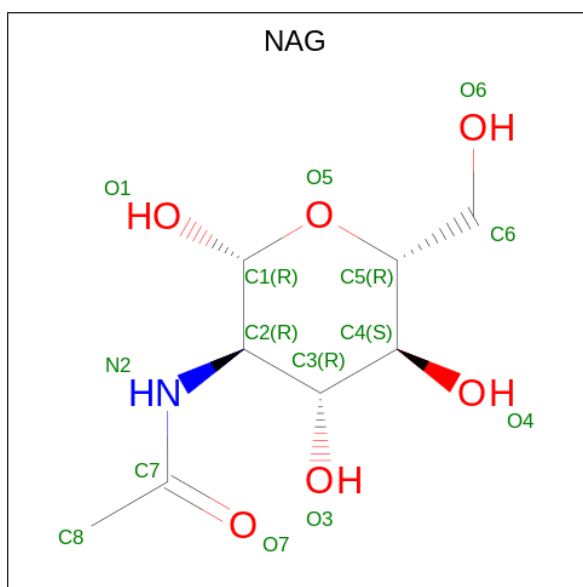
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	2	Total	C	N	O		0	0
			28	16	2	10			
4	E	2	Total	C	N	O		0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (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	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	

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





- Molecule 1: Spike glycoprotein

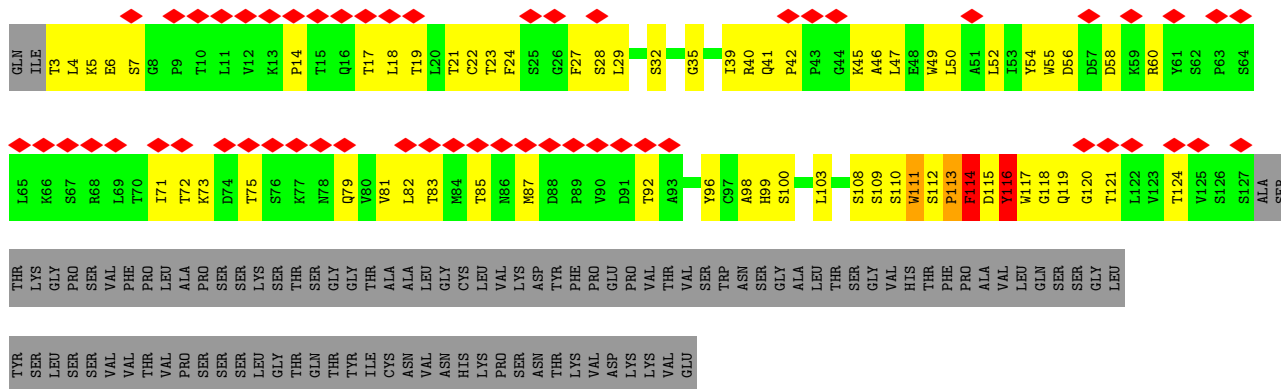
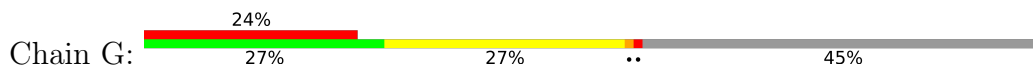


LYS	GLY	ASP	S975	GLY	Y674	Q564	Q474	R403	THR	T167	V83	MET
LEU	PHE	VAL	V976	ILE	Q675	R567	A475	G404	ALA	F168		
ILE	LYS	ASP	L981	GLN	T676	D568	GLN	D405	GLY		N87	VAL
ILE	GLY	LEU	L981	THR	THR	I569	THR	E406	ALA	S172	D88	VAL
VAL	TTR	ASP	L984	ASN	ASN		PRO	Y607	ALA	GLN	Y91	LEU
MET	GLY	ILE		SER	SER	T573	CYS	R408		PHE		VAL
VAL	ASP	SER	E988	PRO	PRO	D574	ASN	Q409	R273	LEU	T95	LEU
THR	CYS	GLY		ARG	ARG	A575	GLY	T415	K278	MET	E96	PRO
ILE	LEU	ILE	Q992	ARG	ARG	V576	VAL	K415	ASP	LEU	K97	LEU
MET	GLY	ASN		ALA	ALA	R577	GLY	Q416	LEU	GLY	S98	VAL
LEU	ASP	ALA	S1030	ARG	ARG		PHE	K417	E281	LEU	N99	SER
CYS	SER	VAL	E1031	SER	SER	L582		I418		GLY		SER
CYS	ILE	VAL	C1032	VAL	VAL	E583	N487	1418	T307	GLY	I105	GLN
MET	ALA	ALA		ALA	ALA	I584		N422	LYS	GLN		CYS
THR	ASP	ASN	S1037	SER	SER	V597	F490	Y423	F318	GLN		GLY
SER	ARG	ILE		ARG	Q690		F491	K424	ASN	ASN	T108	VAL
CYS	LEU	GLN	V1040	LEU	S691	L492	L492		V327	PHE	T109	ASN
CYS	LYS	LYS	D1041	ILE	1692	Q493	Q493	T430	R328	K187	L110	LEU
SER	GLY	GLY		CYS		S494	S494	G431			D111	THR
CYS	ILE	ILE	K1045	ALA		N603	Y495	C432	N331	E191	K113	ARG
LEU	ASP	ASP		GLN	S698		G496	V433	I332			THR
LYS	ARG	ARG	S1051	K354	S704	N606	F497	I434	T333	D198	S116	GLN
GLY	F855	LEU		F855		Q607	GLN	I434	N334	G199		LEU
CYS	N856	LEU	G1059		N710	V608	PRO	N437	V341	V120		PRO
SER	VAL	VAL	H1064	E868	A713	V615	THR	N439	F342	S205	N121	PRO
CYS	ALA	ALA				N616	ASN	S438	K206	K206	N122	
GLY	LYS	LYS	N1074	L878	T719	C617	GLY	N440	H207	A123		
SER	ASN	ASN					V503	I441	T345	T208	T124	
CYS	LEU	LEU	V1094	T883	V722	T618	ASP	ASP			V127	N30
CYS	ASN	ASN				E619	LYS	LYS	V350	N211		S31
LYS	GLY	GLY	V1104	Q901	V729	V620	GLY	VAL	Y351	L212		A27
PHE	SER	SER			PRO		P507	GLY	A352	V213		Y28
ASP	LEU	LEU	I1114	B905	S746	VAL	S514	GLY	W353	R214	C131	S45
GLU	ILE	ILE	I1115	E748	T747	ALA		ASN	I368	D215	E132	L48
ASP	ASP	ASP	C1126	T912		ILE	P521	TTR	L216	F133	F133	H49
SER	GLN	GLN		L916	S758	ALA	V524	ASN	S369	P217	F135	S50
GLU	GLY	GLY	L1141			ASP	C525	ASN				T51
PRO	LEU	LEU	Q1142	Q926	Q762	GLN	Y451	Y451	D364	I231	G142	Q52
VAL	GLY	GLY	P1143			LEU	T531	L452	S371	G332	V143	D53
LEU	LYS	LYS	D1146	Q935	Q779	THR	M532	R454		I233		F59
LYS	TTR	TTR		SER		THR	L546	R454	T376	T236	TTR	S60
GLY	GLN	GLN	SER	S939	K786	TRP	N532	L455	F377	R237	LYS	
VAL	GLY	GLY	PHE	THR	Q787	TRP	V534	F456	C378	Q338	ASN	A67
LYS	TTR	TTR	LYS	THR	I788	ARG	F541	K458	C379	F239	ASN	ILE
LEU	ILE	ILE	GLY	ALA	V789	VAL	M542	S459	Y380	Q239	ASN	H15
HIS	GLY	LYS	GLU	ALA	K790	THR	L461	R460	G381	T240	LYS	VAL
TTR	LEU	TTR	LEU	SER	P791	T638	L547	L461	V382		SER	SER
THR	ASP	ASP	ASP	GLY	P792	6639	T546	K462	T385	TTR	TRP	GLY
LEU	LEU	TTR	LYS	LYS	D808	S640	S555	F465		THR	M153	THR
GLY	TTR	PHE					S556	R466	N388	LEU	E156	ASN
ASP	ILE	ILE					R586	D467		PRO	F157	GLY
TTR	LYS	TTR	LYS	THR	V826	R646	K557	I468	C391	GLY		THR
LYS	ASN	LEU	ASN	THR	THR		K558	S469	V395	ASP	R158	LYS
ASP	GLY	PHE	HIS	GLY	ALA	C649	F559	S469	Y396	SER	V159	ARG
THR	THR	THR	THR	THR	ALA		L560			SER		PHE
ASP	ILE	ILE	SER	ASP	ALA	E661		I472		SER	N164	ASP
ASP	ALA	ALA	PRO	GLY	ALA		C563	Y472	T209	GLY	N81	N82

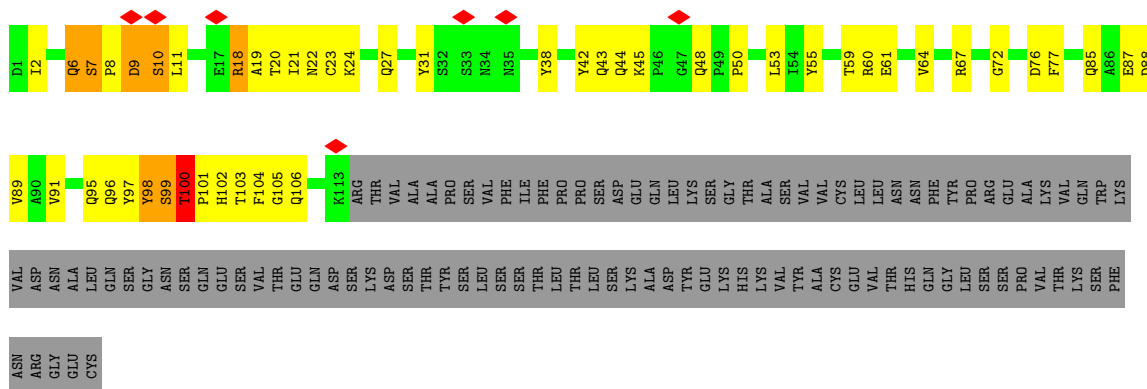
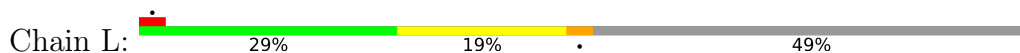
- Molecule 1: Spike glycoprotein



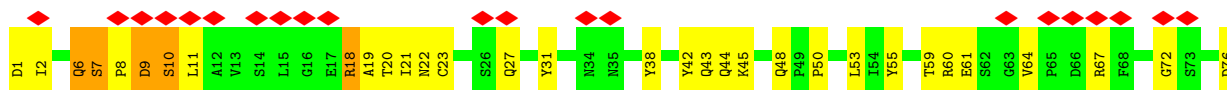
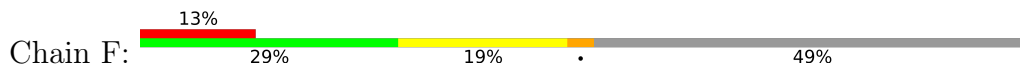
- Molecule 2: Heavy chain of P5A-3C12

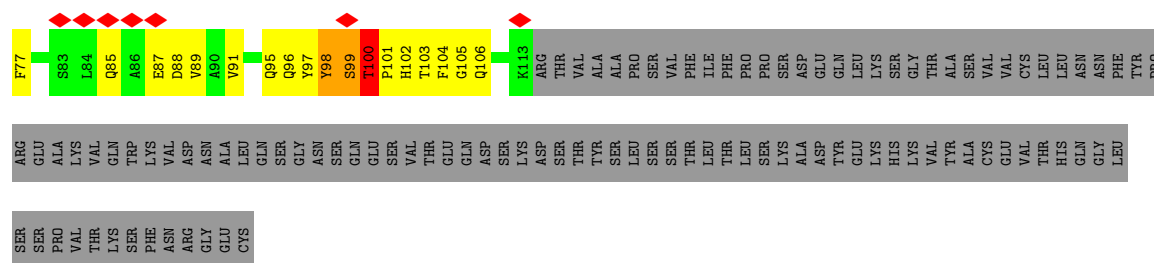


- Molecule 3: Light chain of P5A-3C12



- Molecule 3: Light chain of P5A-3C12





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

Chain D: 50% 50%



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

Chain E: 100%



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

Chain I: 50% 50%



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

Chain J: 50% 50%



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

Chain K: 100%



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

Chain M:  50% 50%



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

Chain N:  100%



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

Chain O:  100%



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

Chain P:  50% 50% 50%



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

Chain Q:  100%



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

Chain R:  50% 50%



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

Chain S:  50% 50%



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

Chain T:  50% 50%



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

Chain U:  100%



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

Chain V:  100%



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

Chain W:  50% 50%



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

Chain X:  50% 50%



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

Chain Y:  50% 50%



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

Chain Z: 

MAG1  
MAG2

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

Chain a: 

MAG1  
MAG2

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

Chain b: 

MAG1  
MAG2

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

Chain c: 

MAG1  
MAG2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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 (6k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0087	Depositor
Map size ( $\text{\AA}$ )	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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	0.59	0/8028	0.55	0/10919
1	B	0.59	0/8039	0.55	0/10936
1	C	0.49	0/7864	0.55	0/10691
2	G	0.36	0/999	0.68	0/1367
2	H	0.36	0/999	0.68	0/1367
3	F	0.38	0/901	0.59	0/1225
3	L	0.38	0/901	0.60	0/1225
All	All	0.54	0/27731	0.56	0/37730

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](#)

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	7853	0	7653	203	0
1	B	7863	0	7658	242	0
1	C	7696	0	7514	147	0
2	G	972	0	956	136	0
2	H	972	0	956	141	0
3	F	880	0	849	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	880	0	849	108	0
4	D	28	0	25	0	0
4	E	28	0	25	3	0
4	I	28	0	25	1	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	1	0
4	N	28	0	25	2	0
4	O	28	0	25	0	0
4	P	28	0	25	1	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	1	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	3	0
4	X	28	0	25	0	0
4	Y	28	0	25	1	0
4	Z	28	0	25	1	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	c	28	0	25	0	0
5	A	112	0	104	2	0
5	B	126	0	117	4	0
5	C	126	0	117	6	0
All	All	28096	0	27323	981	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 18.

The worst 5 of 981 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)
2:H:113:PRO:HA	2:H:117:TRP:CZ2	1.35	1.59
2:G:113:PRO:HA	2:G:117:TRP:CZ2	1.35	1.58
1:B:329:PHE:CD2	1:B:528:LYS:HG3	1.47	1.47
2:G:111:TRP:HD1	3:F:102:HIS:CE1	1.36	1.44
2:H:111:TRP:HD1	3:L:102:HIS:CE1	1.36	1.42

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	986/1283 (77%)	891 (90%)	82 (8%)	13 (1%)	10	39
1	B	988/1283 (77%)	889 (90%)	93 (9%)	6 (1%)	22	55
1	C	958/1283 (75%)	868 (91%)	89 (9%)	1 (0%)	48	79
2	G	123/226 (54%)	102 (83%)	18 (15%)	3 (2%)	5	29
2	H	123/226 (54%)	102 (83%)	18 (15%)	3 (2%)	5	29
3	F	111/220 (50%)	92 (83%)	13 (12%)	6 (5%)	1	17
3	L	111/220 (50%)	92 (83%)	13 (12%)	6 (5%)	1	17
All	All	3400/4741 (72%)	3036 (89%)	326 (10%)	38 (1%)	15	42

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	LEU
1	A	529	LYS
1	A	814	LYS
2	H	113	PRO
2	H	114	PHE

### 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	879/1122 (78%)	789 (90%)	90 (10%)	6	24
1	B	881/1122 (78%)	783 (89%)	98 (11%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	862/1122 (77%)	762 (88%)	100 (12%)	4	21
2	G	112/199 (56%)	107 (96%)	5 (4%)	23	47
2	H	112/199 (56%)	107 (96%)	5 (4%)	23	47
3	F	99/195 (51%)	95 (96%)	4 (4%)	27	50
3	L	99/195 (51%)	95 (96%)	4 (4%)	27	50
All	All	3044/4154 (73%)	2738 (90%)	306 (10%)	9	24

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	328	ARG
1	B	937	SER
1	B	375	SER
1	B	576	VAL
1	B	1123	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	102	HIS
1	B	498	GLN
3	F	6	GLN
1	B	188	ASN
1	B	658	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

44 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	1,4	14,14,15	0.41	0	17,19,21	0.57	0
4	NAG	D	2	4	14,14,15	0.27	0	17,19,21	0.61	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.57	0	17,19,21	0.57	0
4	NAG	E	2	4	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	I	1	1,4	14,14,15	0.23	0	17,19,21	1.35	1 (5%)
4	NAG	I	2	4	14,14,15	0.19	0	17,19,21	0.50	0
4	NAG	J	1	1,4	14,14,15	0.52	0	17,19,21	0.70	1 (5%)
4	NAG	J	2	4	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	K	1	1,4	14,14,15	0.34	0	17,19,21	0.41	0
4	NAG	K	2	4	14,14,15	0.20	0	17,19,21	0.73	0
4	NAG	M	1	1,4	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	M	2	4	14,14,15	0.57	0	17,19,21	1.32	1 (5%)
4	NAG	N	1	1,4	14,14,15	0.65	1 (7%)	17,19,21	0.44	0
4	NAG	N	2	4	14,14,15	0.31	0	17,19,21	1.36	2 (11%)
4	NAG	O	1	1,4	14,14,15	0.42	0	17,19,21	0.43	0
4	NAG	O	2	4	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	P	1	1,4	14,14,15	0.30	0	17,19,21	0.41	0
4	NAG	P	2	4	14,14,15	0.16	0	17,19,21	0.48	0
4	NAG	Q	1	1,4	14,14,15	0.32	0	17,19,21	0.40	0
4	NAG	Q	2	4	14,14,15	0.37	0	17,19,21	0.36	0
4	NAG	R	1	1,4	14,14,15	0.35	0	17,19,21	1.11	1 (5%)
4	NAG	R	2	4	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	S	1	1,4	14,14,15	0.29	0	17,19,21	0.69	1 (5%)
4	NAG	S	2	4	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	T	1	1,4	14,14,15	0.74	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	T	2	4	14,14,15	0.29	0	17,19,21	0.68	0
4	NAG	U	1	1,4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	U	2	4	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	V	1	1,4	14,14,15	0.52	0	17,19,21	0.50	0
4	NAG	V	2	4	14,14,15	0.27	0	17,19,21	0.59	0
4	NAG	W	1	1,4	14,14,15	0.59	1 (7%)	17,19,21	0.56	0
4	NAG	W	2	4	14,14,15	0.29	0	17,19,21	0.46	0
4	NAG	X	1	1,4	14,14,15	0.33	0	17,19,21	0.63	1 (5%)

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	0.52	0	17,19,21	0.46	0
4	NAG	Y	1	1,4	14,14,15	0.38	0	17,19,21	0.72	0
4	NAG	Y	2	4	14,14,15	0.30	0	17,19,21	1.31	2 (11%)
4	NAG	Z	1	1,4	14,14,15	0.70	1 (7%)	17,19,21	0.69	0
4	NAG	Z	2	4	14,14,15	0.40	0	17,19,21	1.40	3 (17%)
4	NAG	a	1	1,4	14,14,15	0.70	1 (7%)	17,19,21	0.66	0
4	NAG	a	2	4	14,14,15	0.30	0	17,19,21	0.63	0
4	NAG	b	1	1,4	14,14,15	0.24	0	17,19,21	0.69	1 (5%)
4	NAG	b	2	4	14,14,15	0.16	0	17,19,21	0.46	0
4	NAG	c	1	1,4	14,14,15	0.40	0	17,19,21	1.16	2 (11%)
4	NAG	c	2	4	14,14,15	0.34	0	17,19,21	0.41	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	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	5/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	1	NAG	O5-C1	-2.69	1.39	1.43
4	a	1	NAG	O5-C1	-2.55	1.39	1.43
4	Z	1	NAG	O5-C1	-2.36	1.39	1.43
4	N	1	NAG	O5-C1	-2.19	1.40	1.43
4	W	1	NAG	O5-C1	-2.06	1.40	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C2-N2-C7	4.64	129.51	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Z	2	NAG	C2-N2-C7	4.37	129.13	122.90
4	N	2	NAG	C2-N2-C7	4.36	129.12	122.90
4	M	2	NAG	C2-N2-C7	4.35	129.10	122.90
4	Y	2	NAG	C2-N2-C7	4.34	129.09	122.90

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

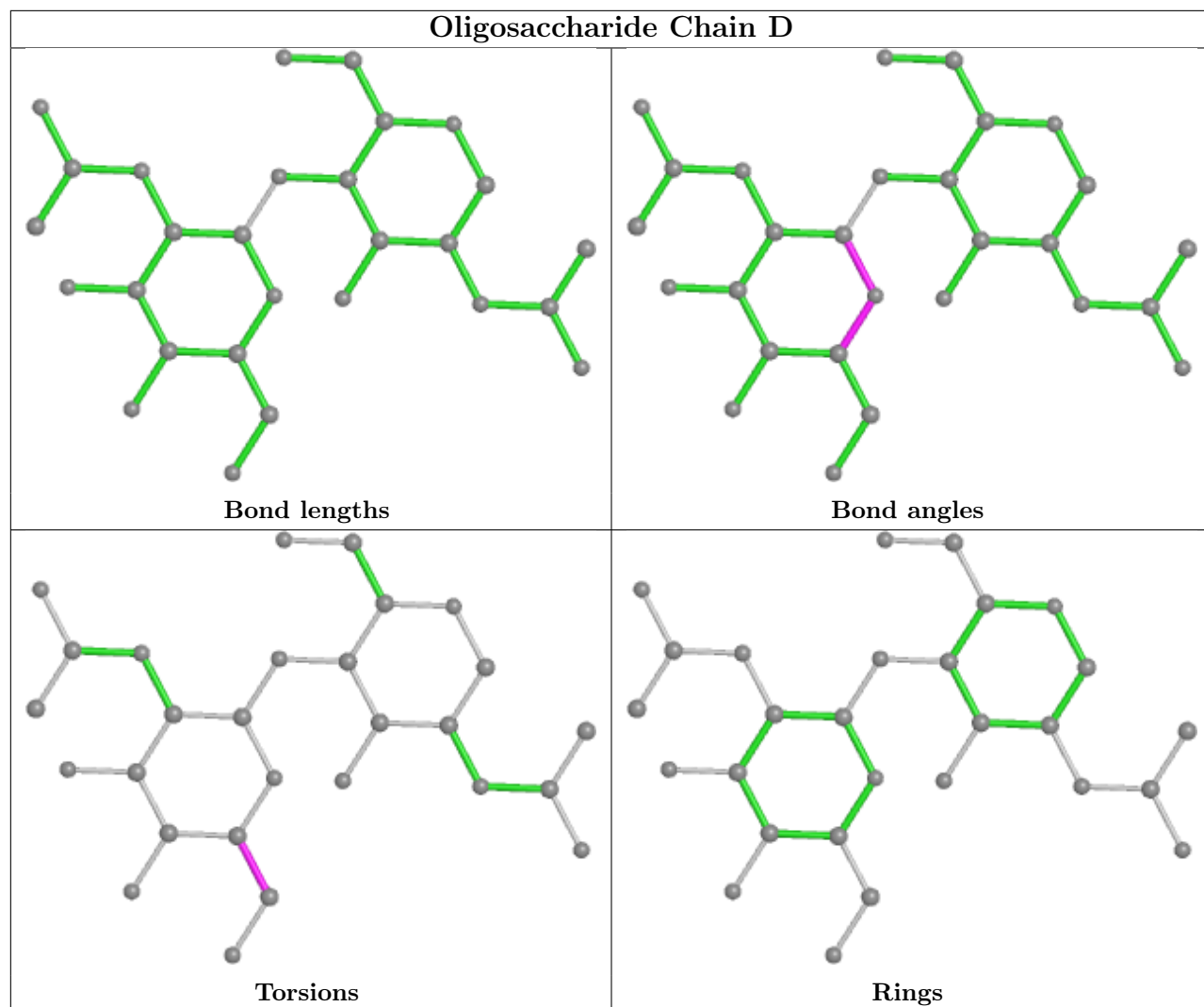
Mol	Chain	Res	Type	Atoms
4	I	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6

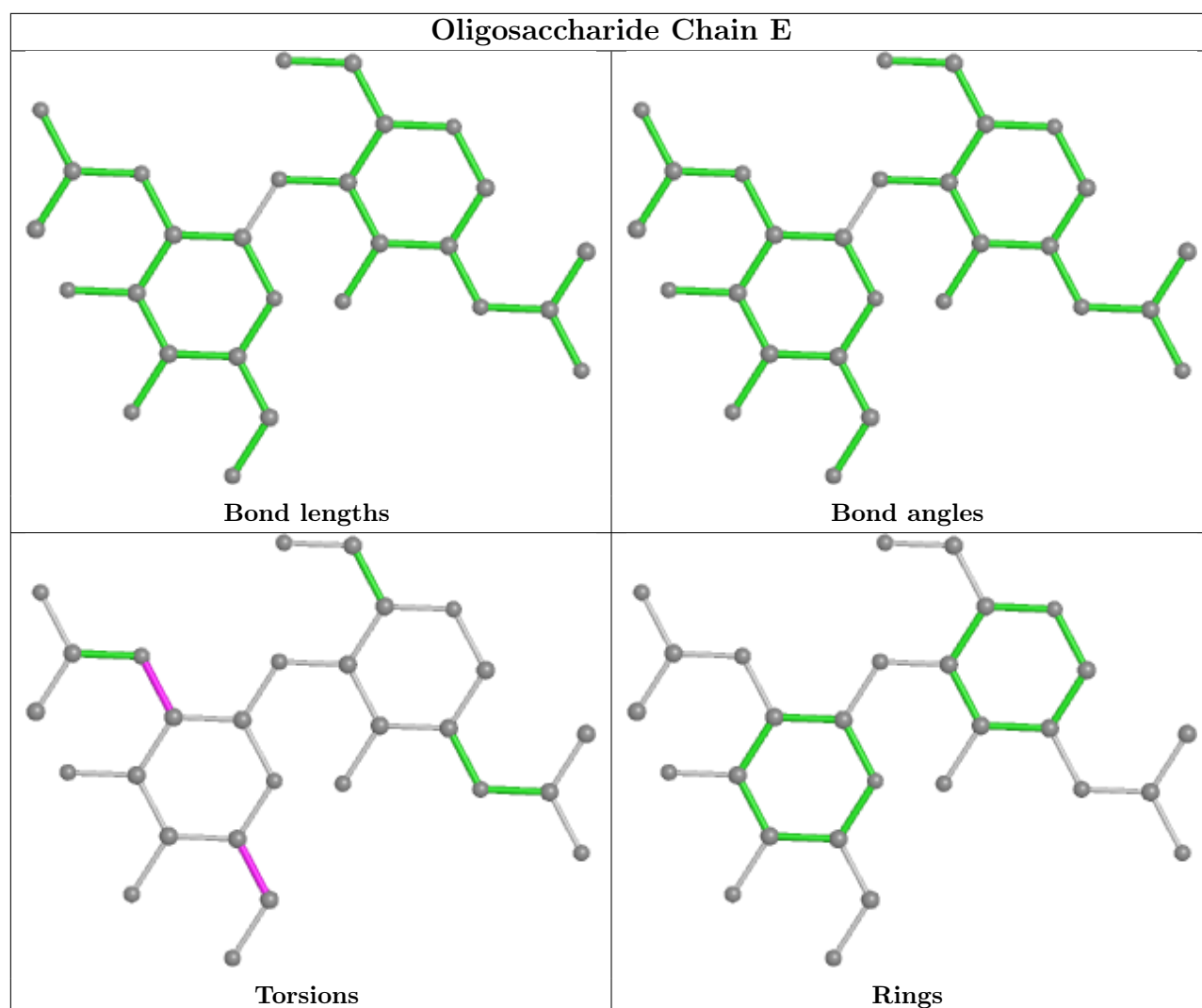
There are no ring outliers.

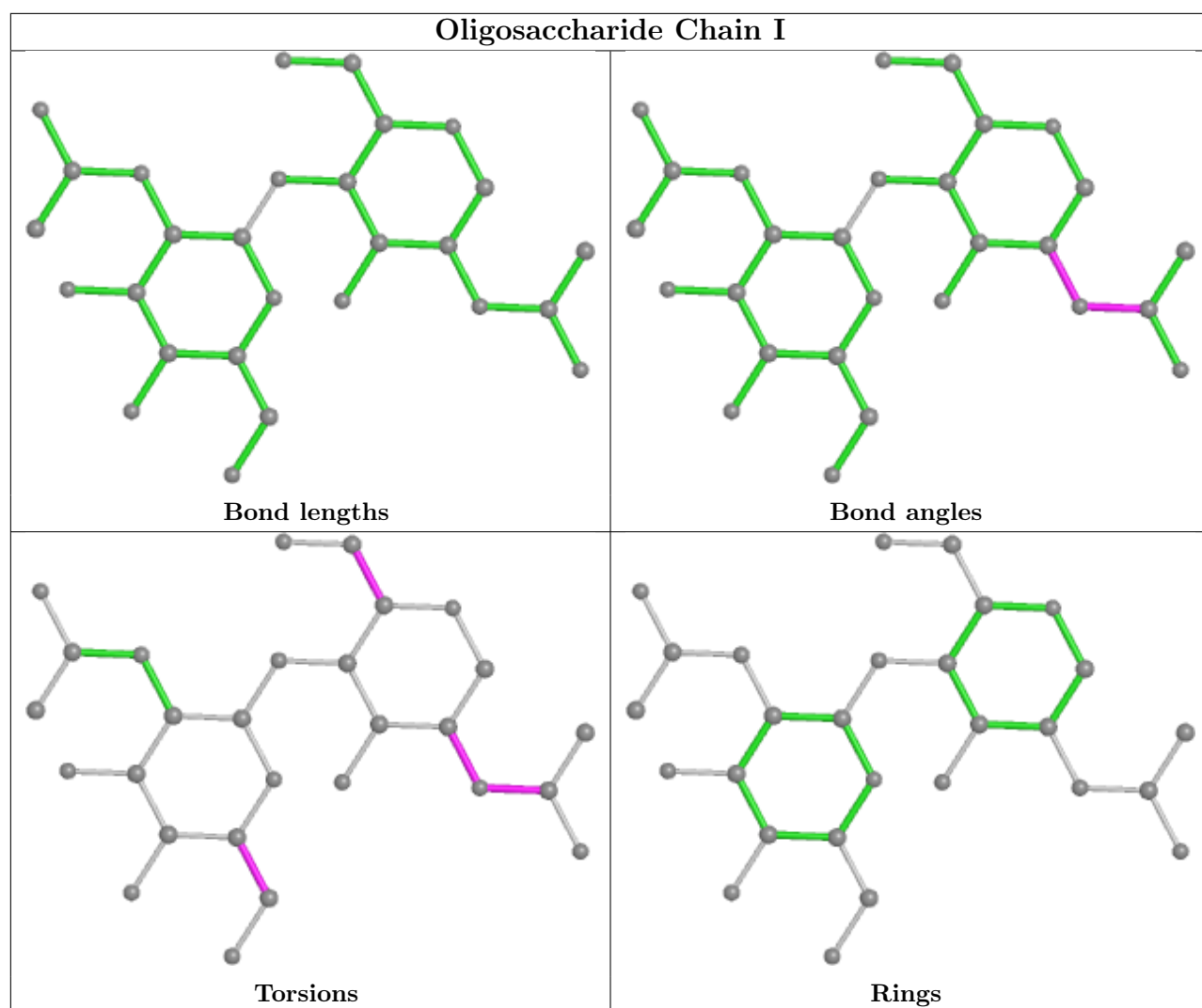
13 monomers are involved in 14 short contacts:

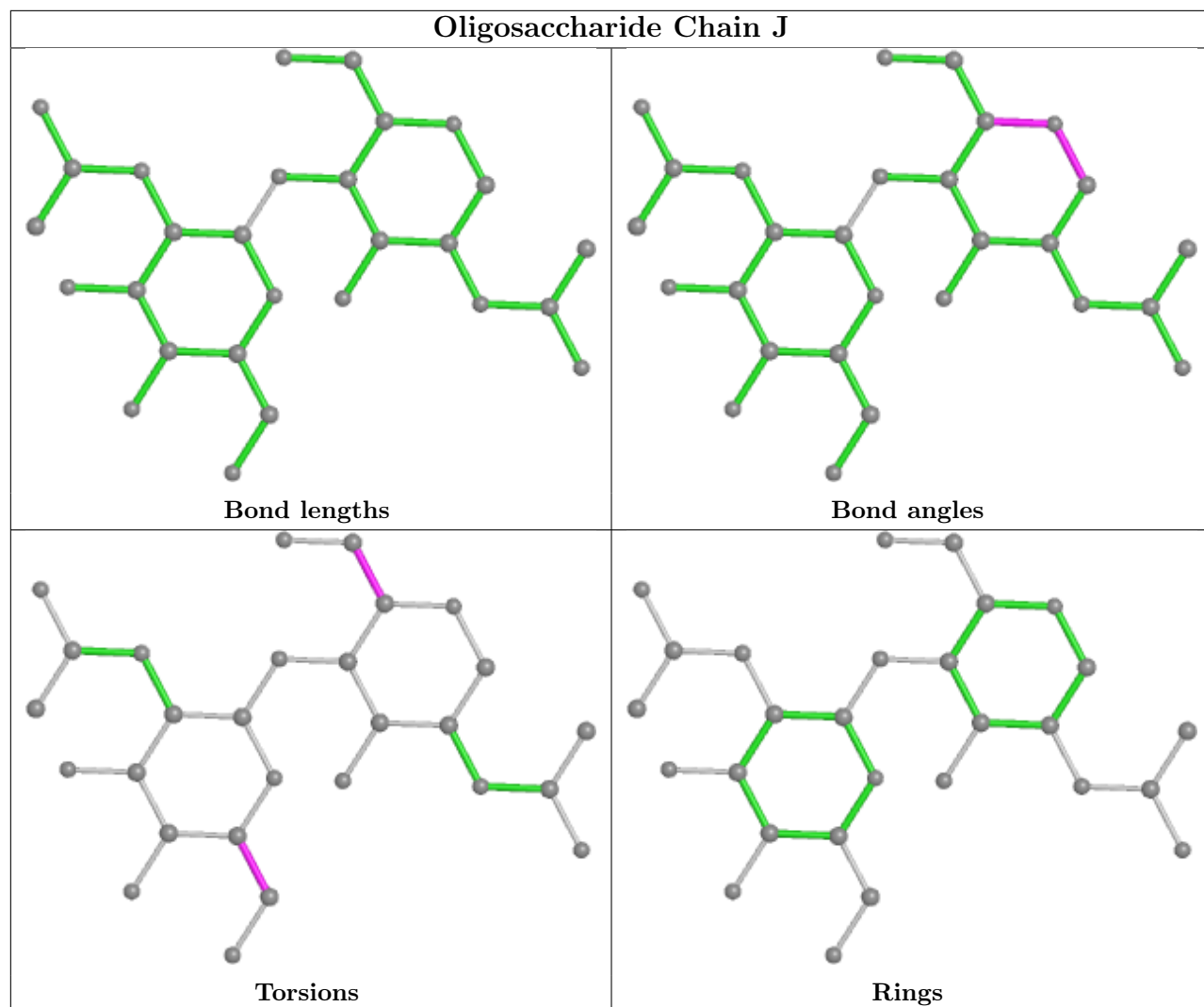
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	W	1	NAG	3	0
4	P	1	NAG	1	0
4	N	1	NAG	1	0
4	Y	2	NAG	1	0
4	E	1	NAG	3	0
4	E	2	NAG	2	0
4	I	1	NAG	1	0
4	T	2	NAG	1	0
4	N	2	NAG	1	0
4	W	2	NAG	2	0
4	T	1	NAG	1	0
4	M	2	NAG	1	0
4	Z	2	NAG	1	0

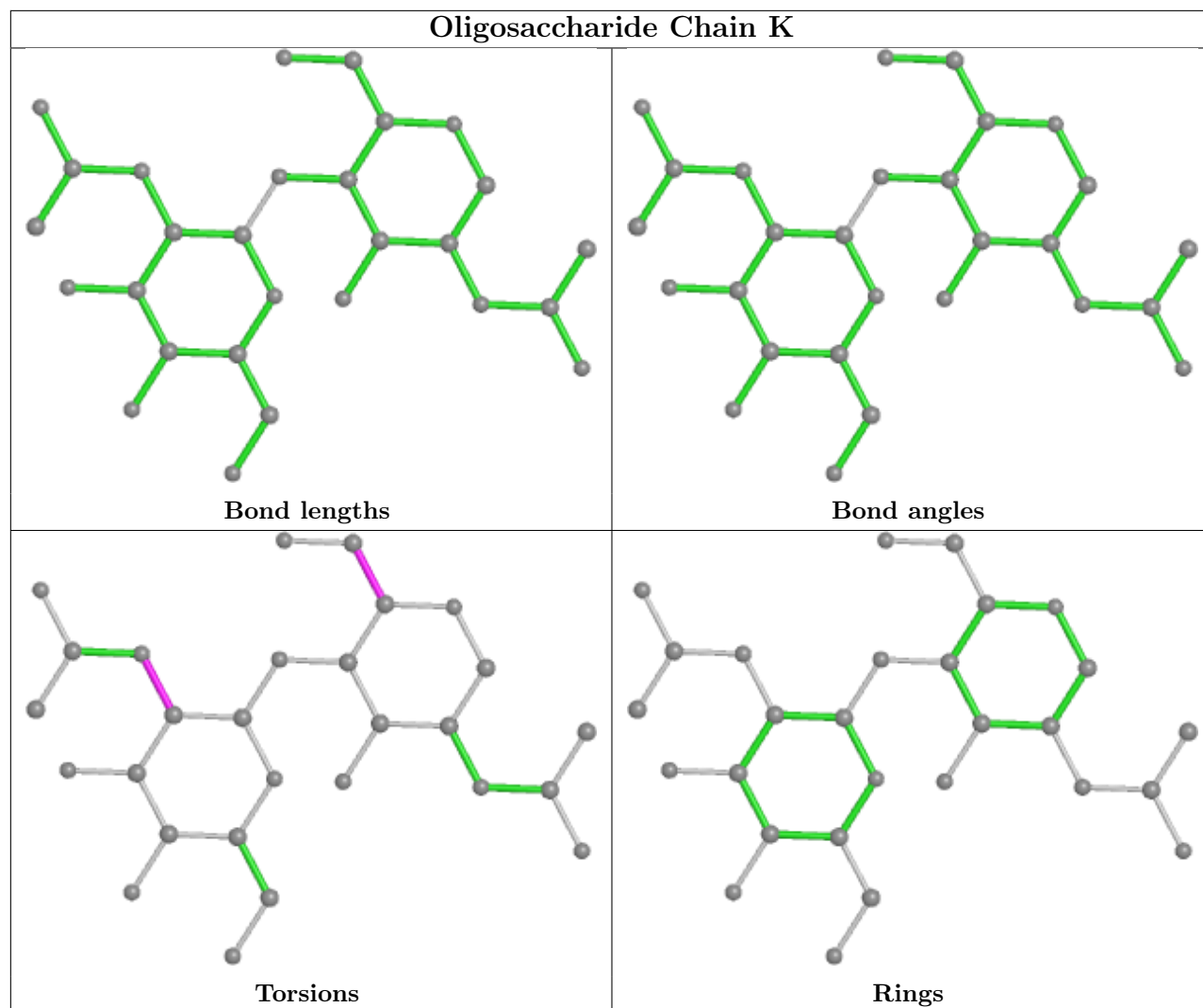
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

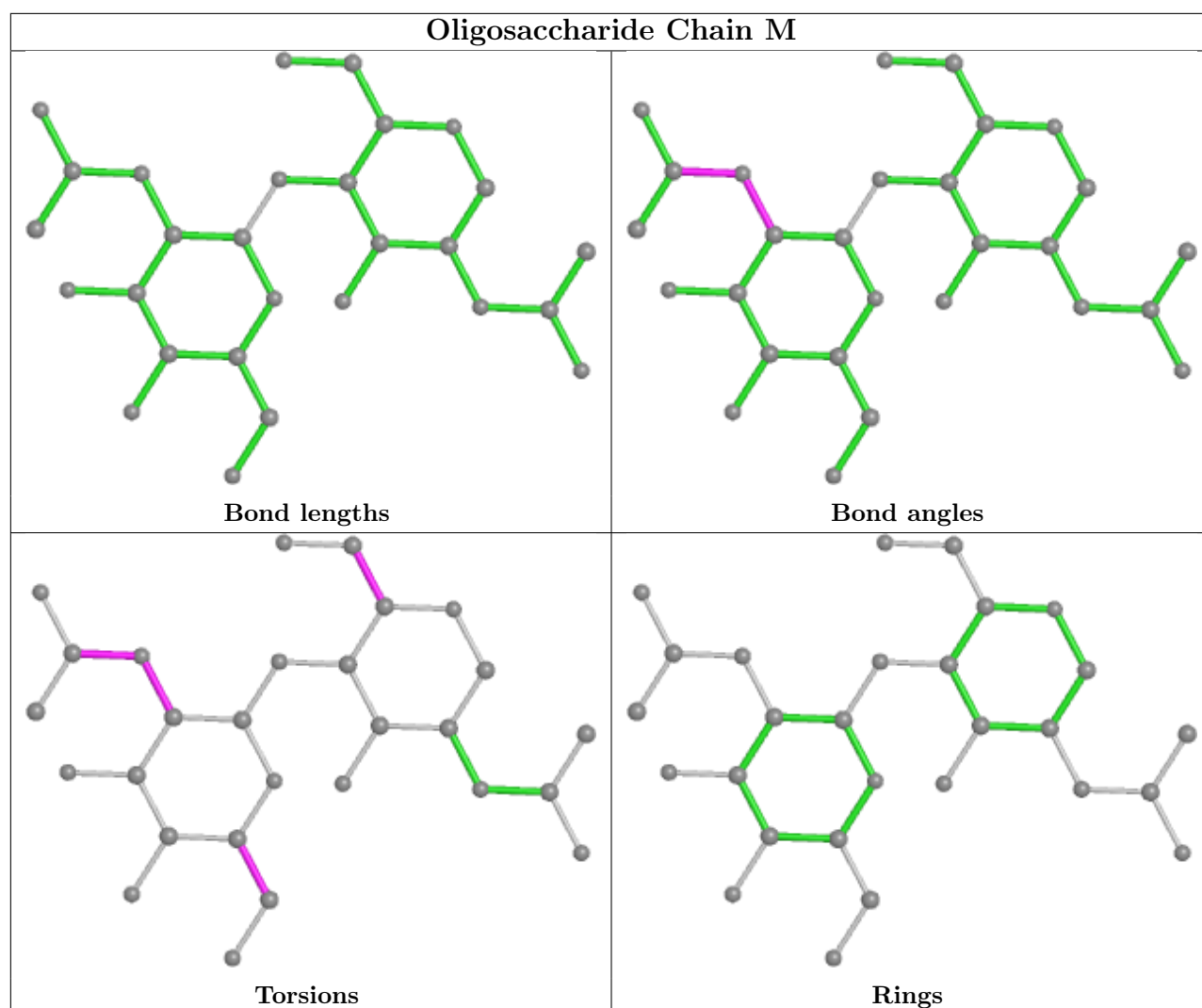


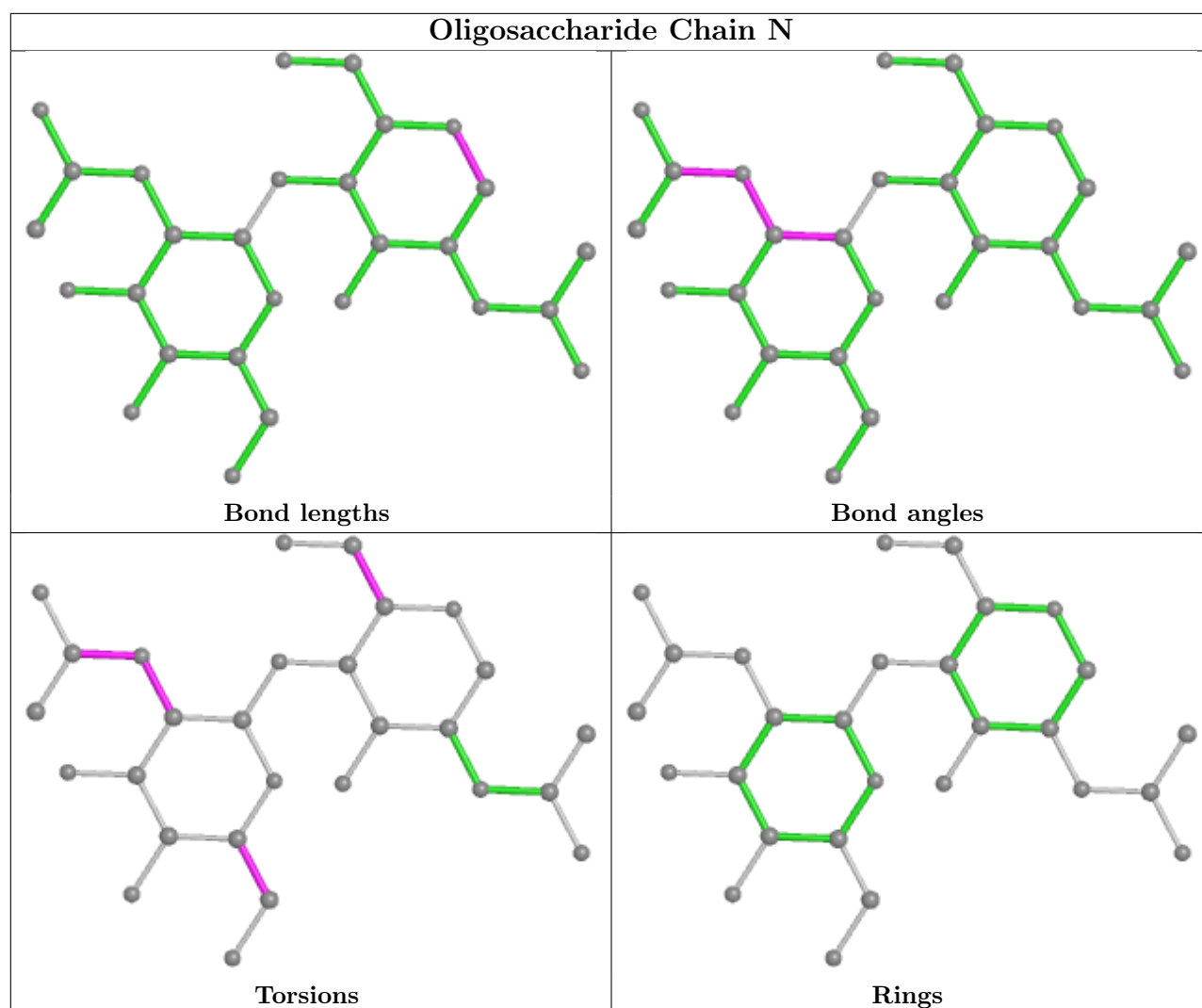




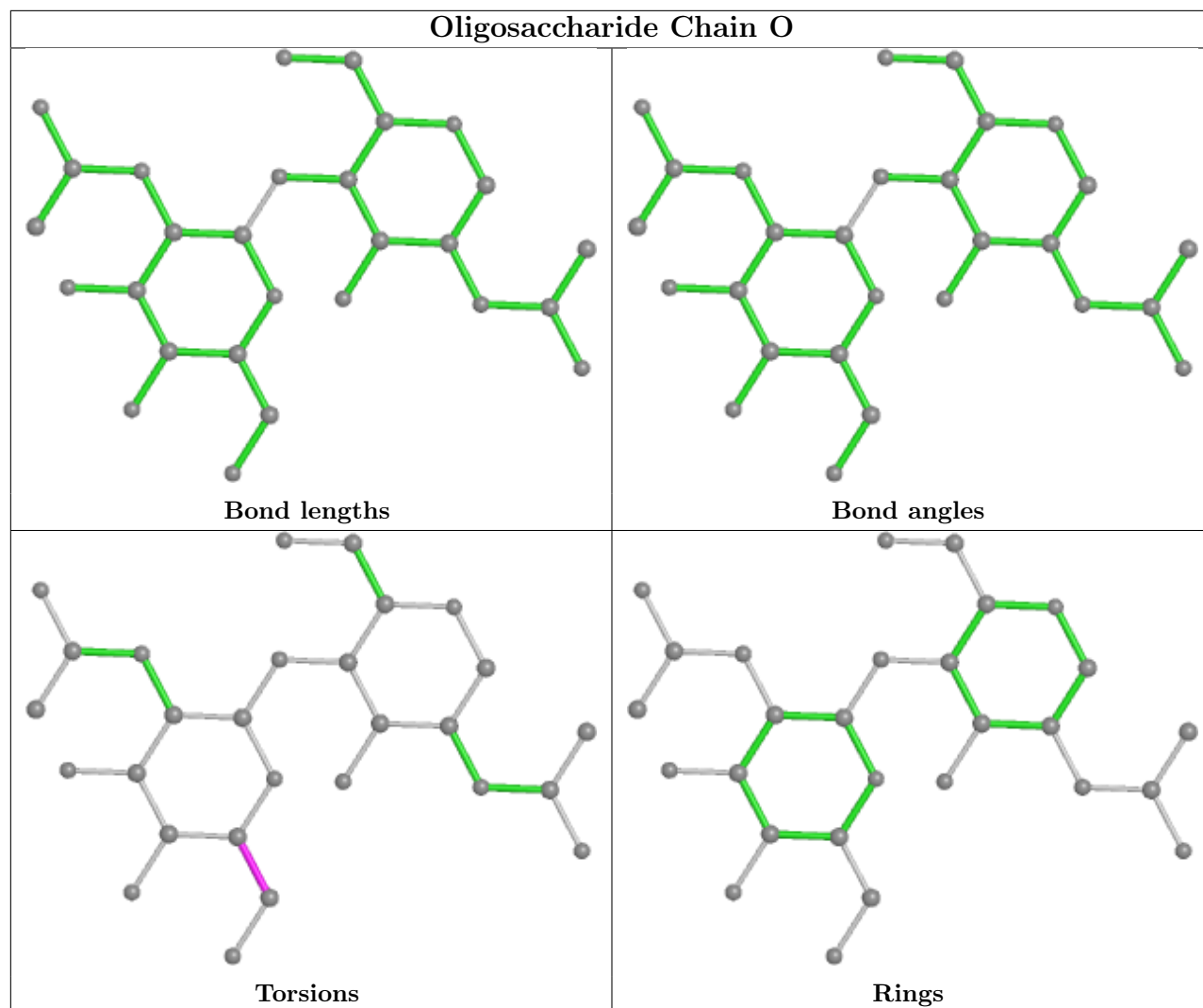


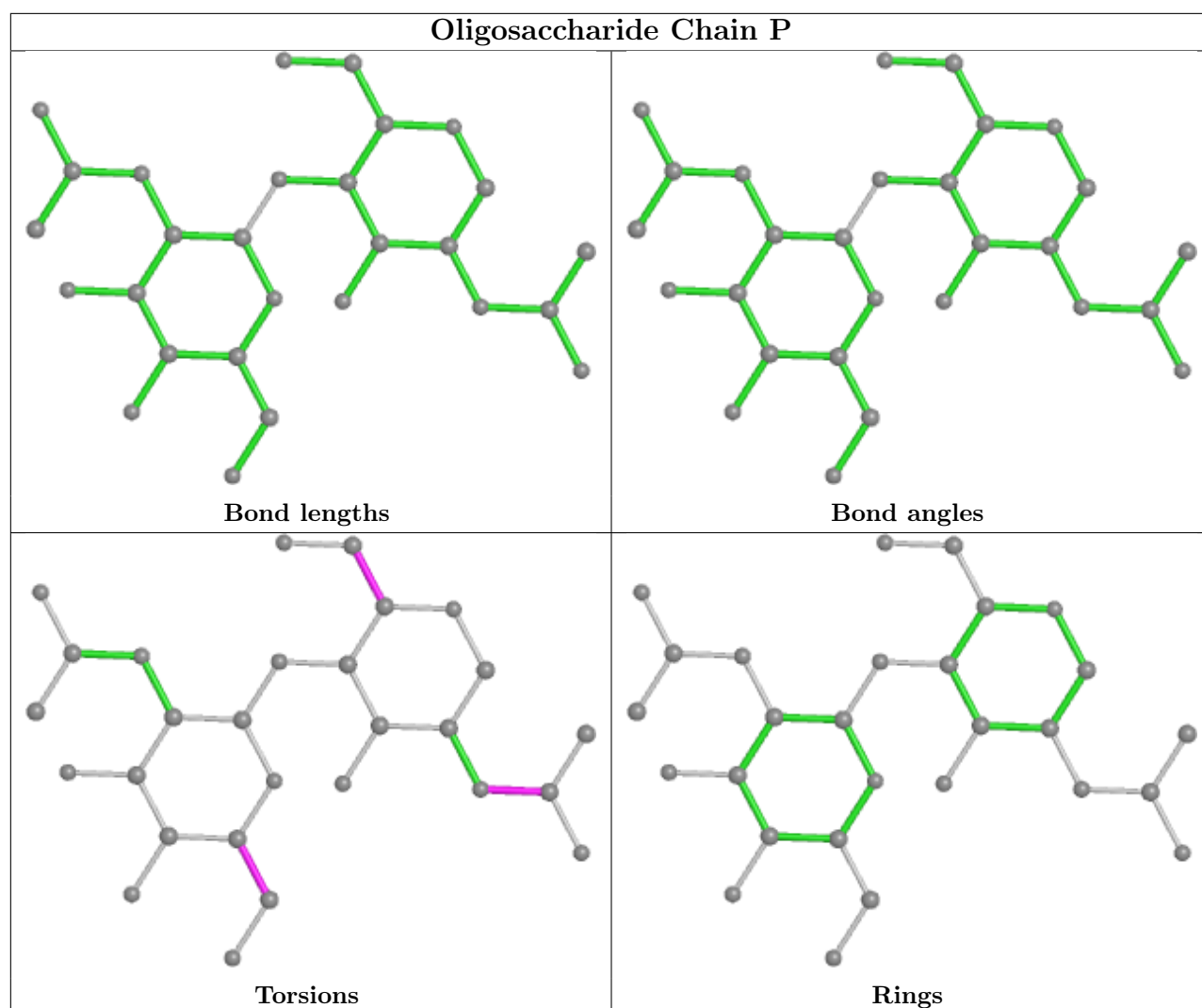


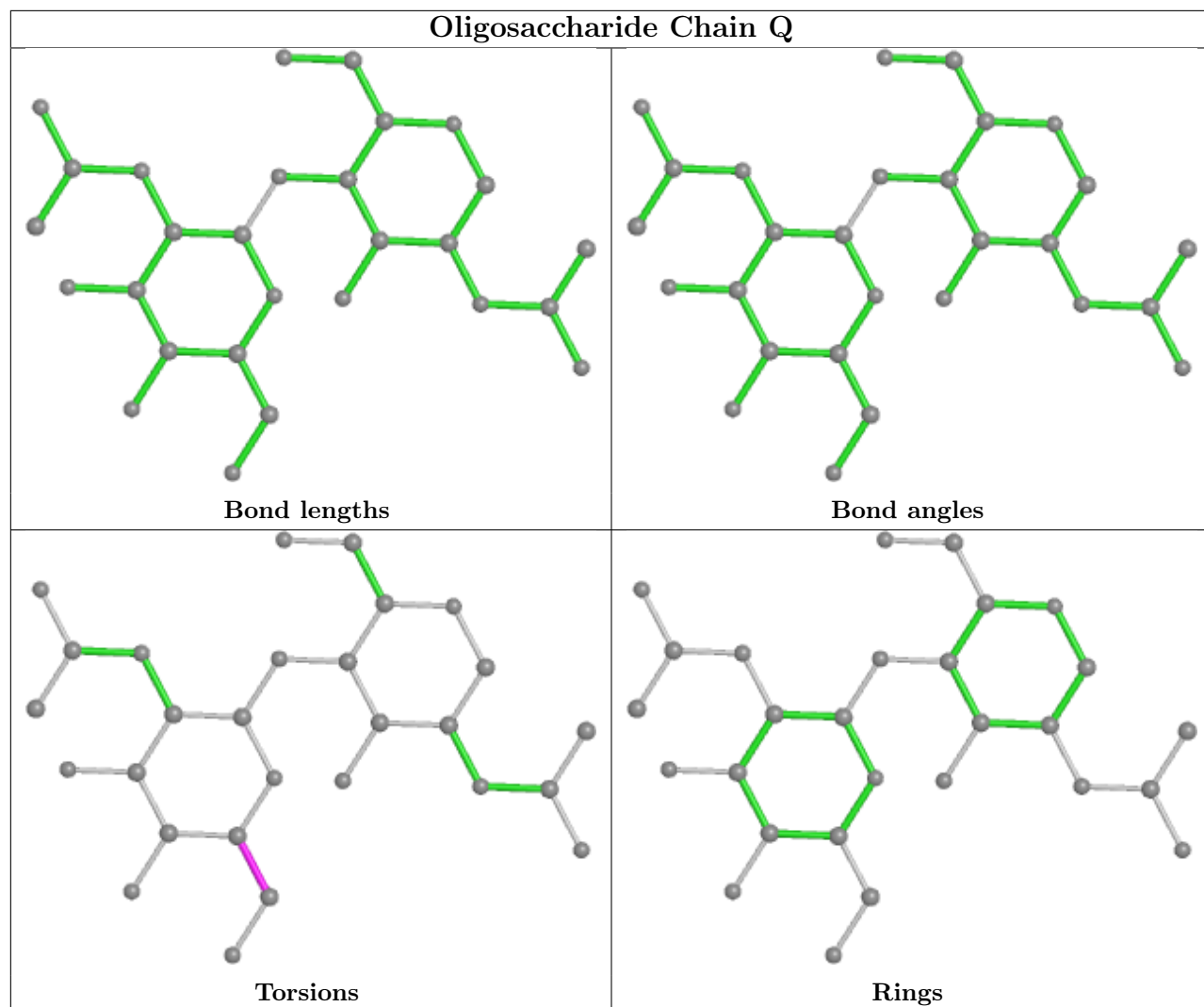


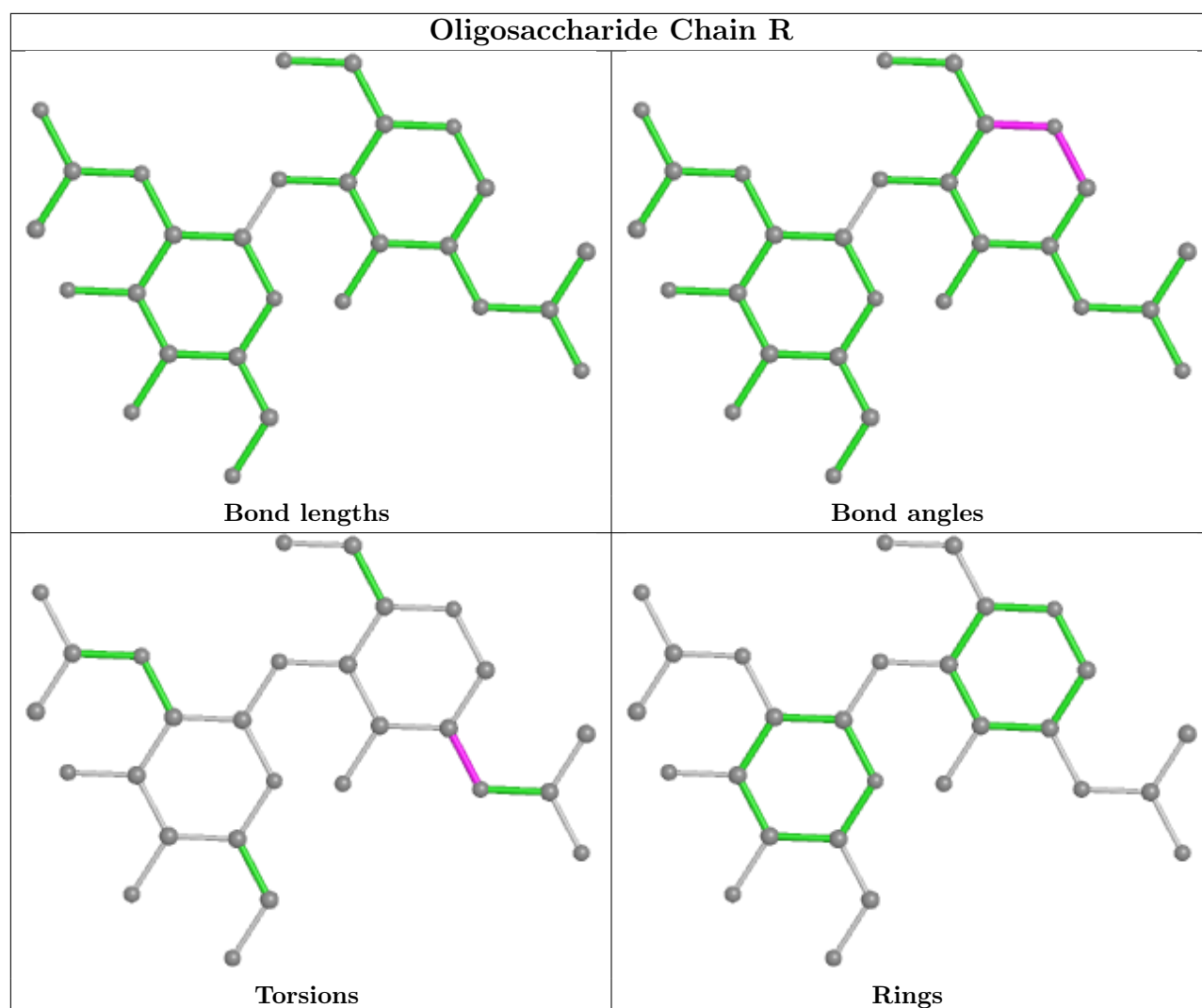


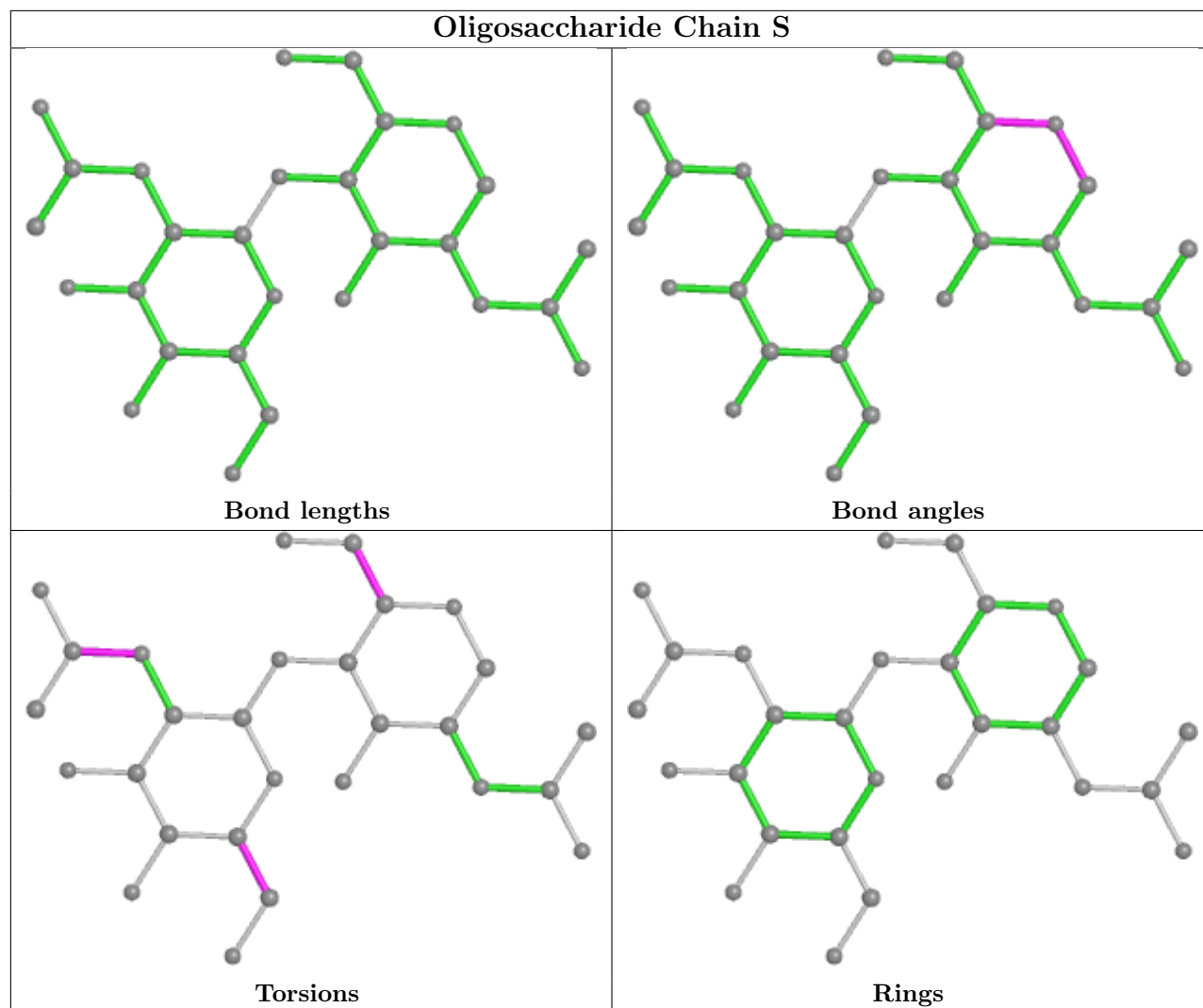


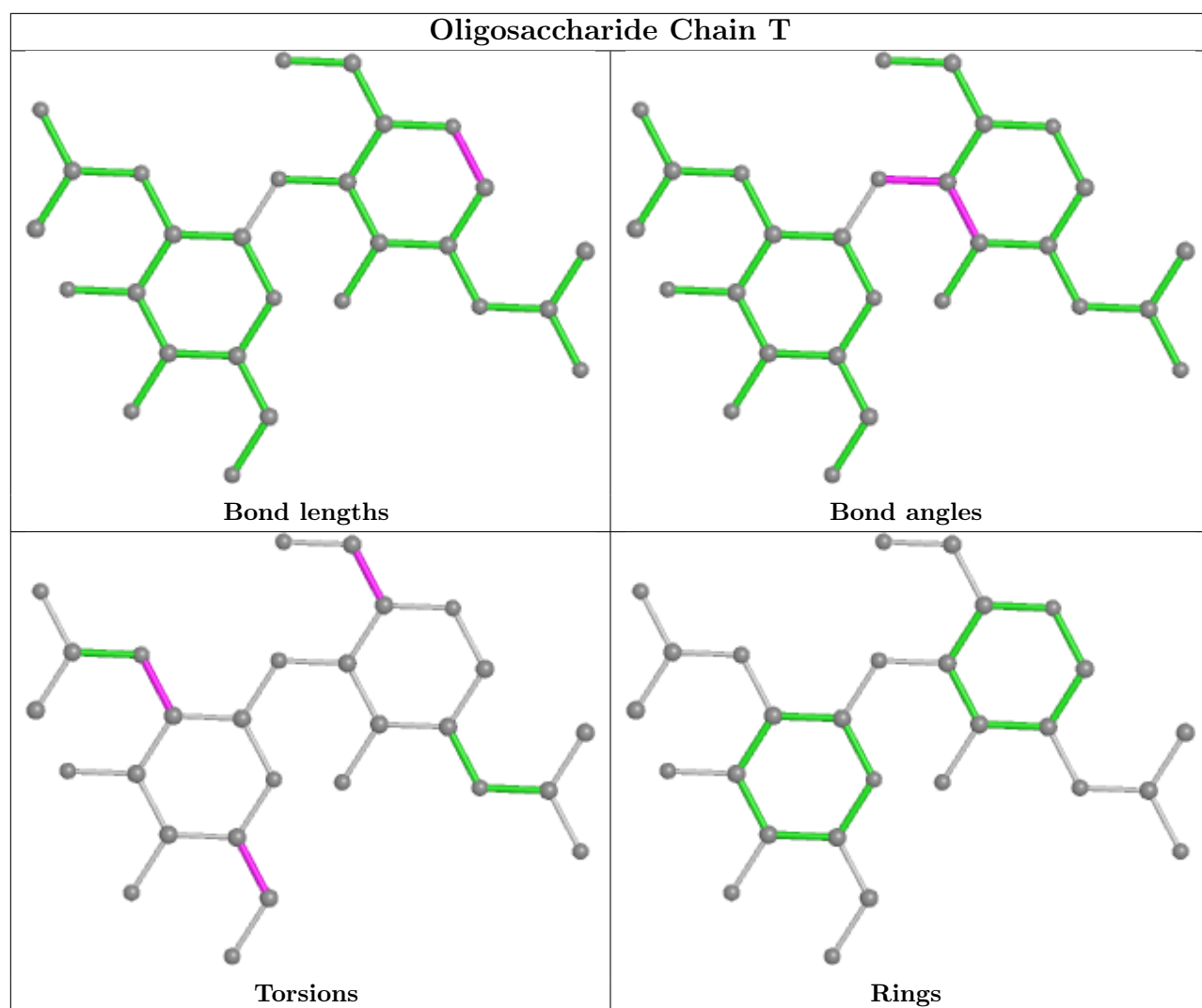


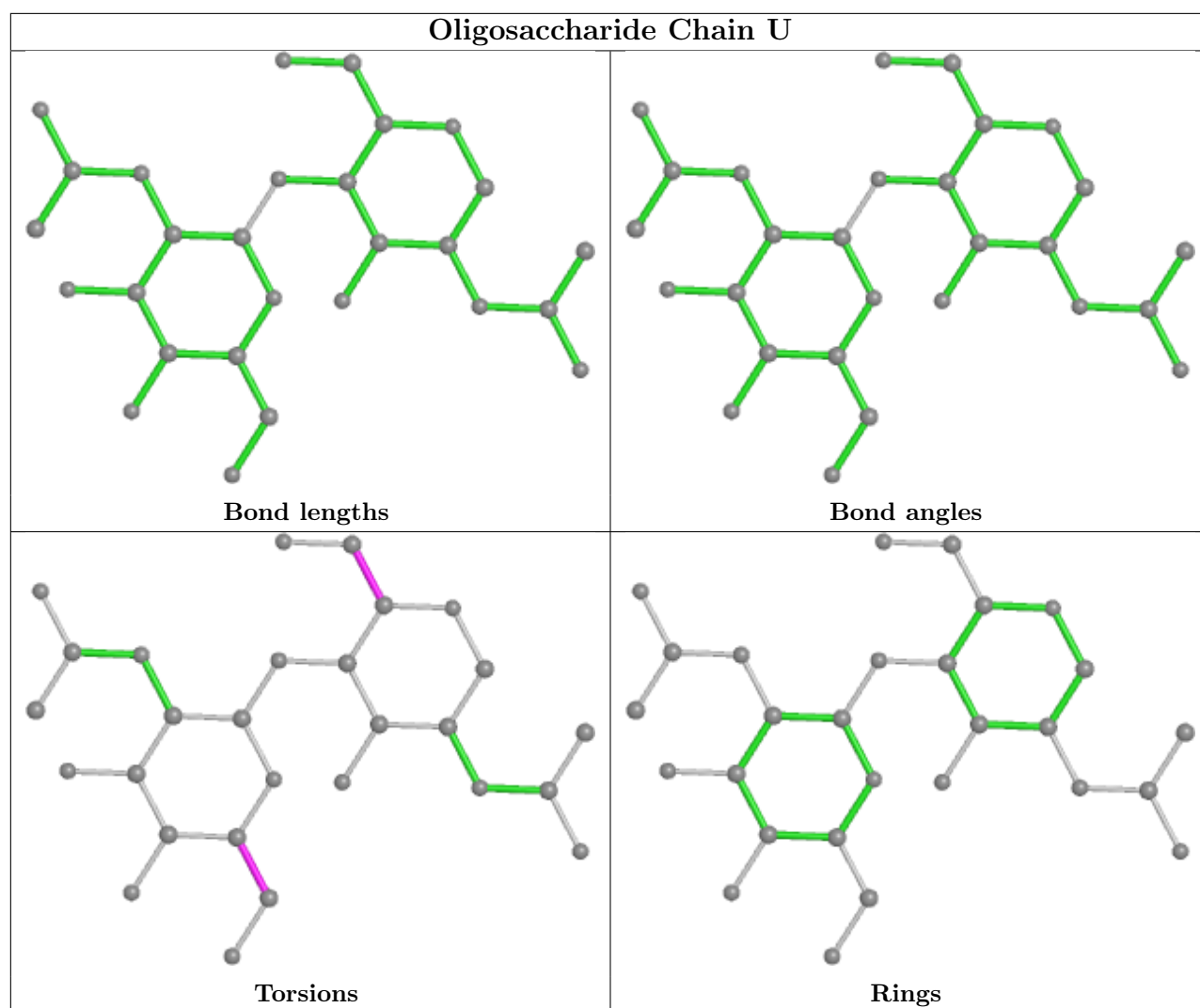


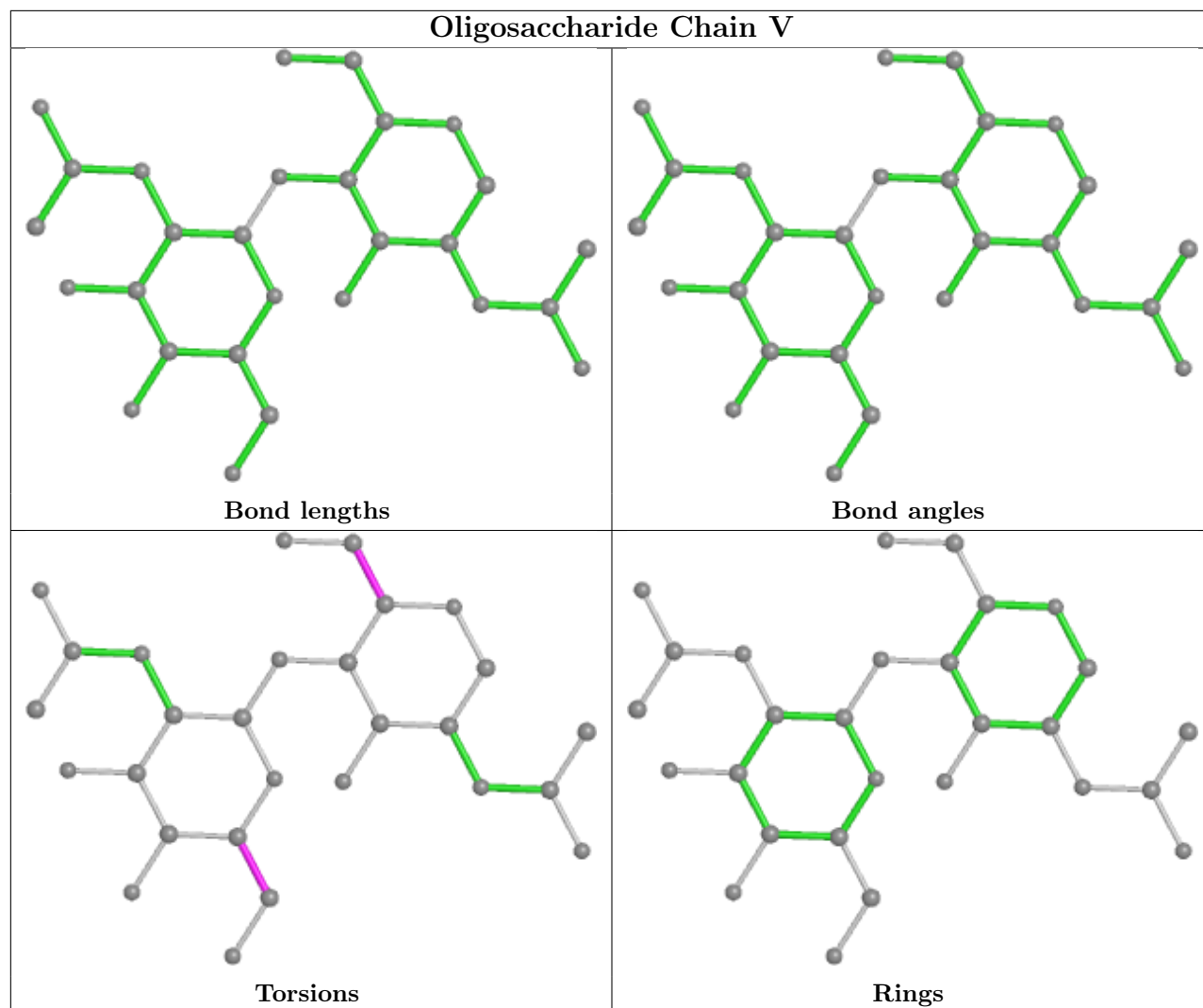




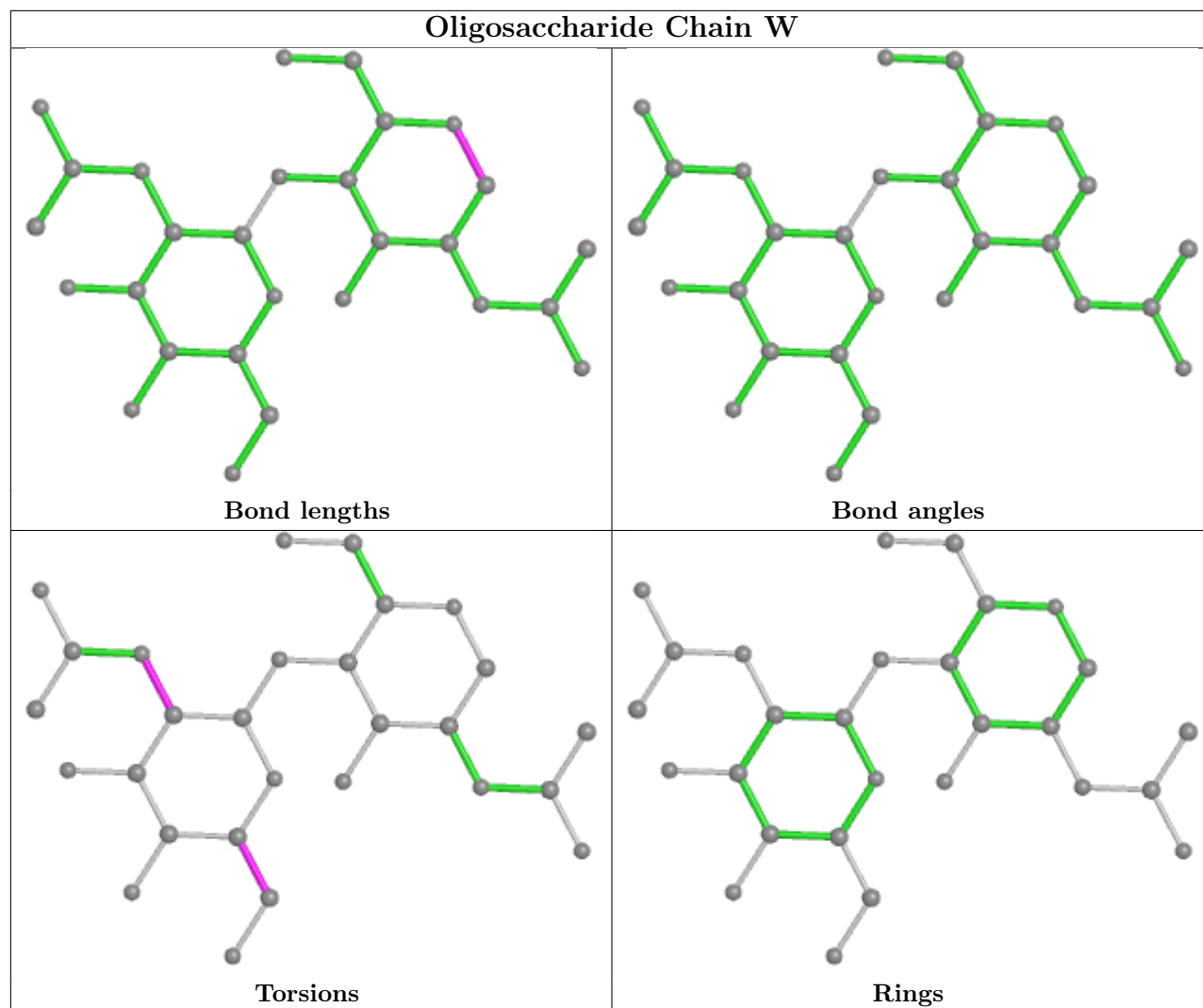


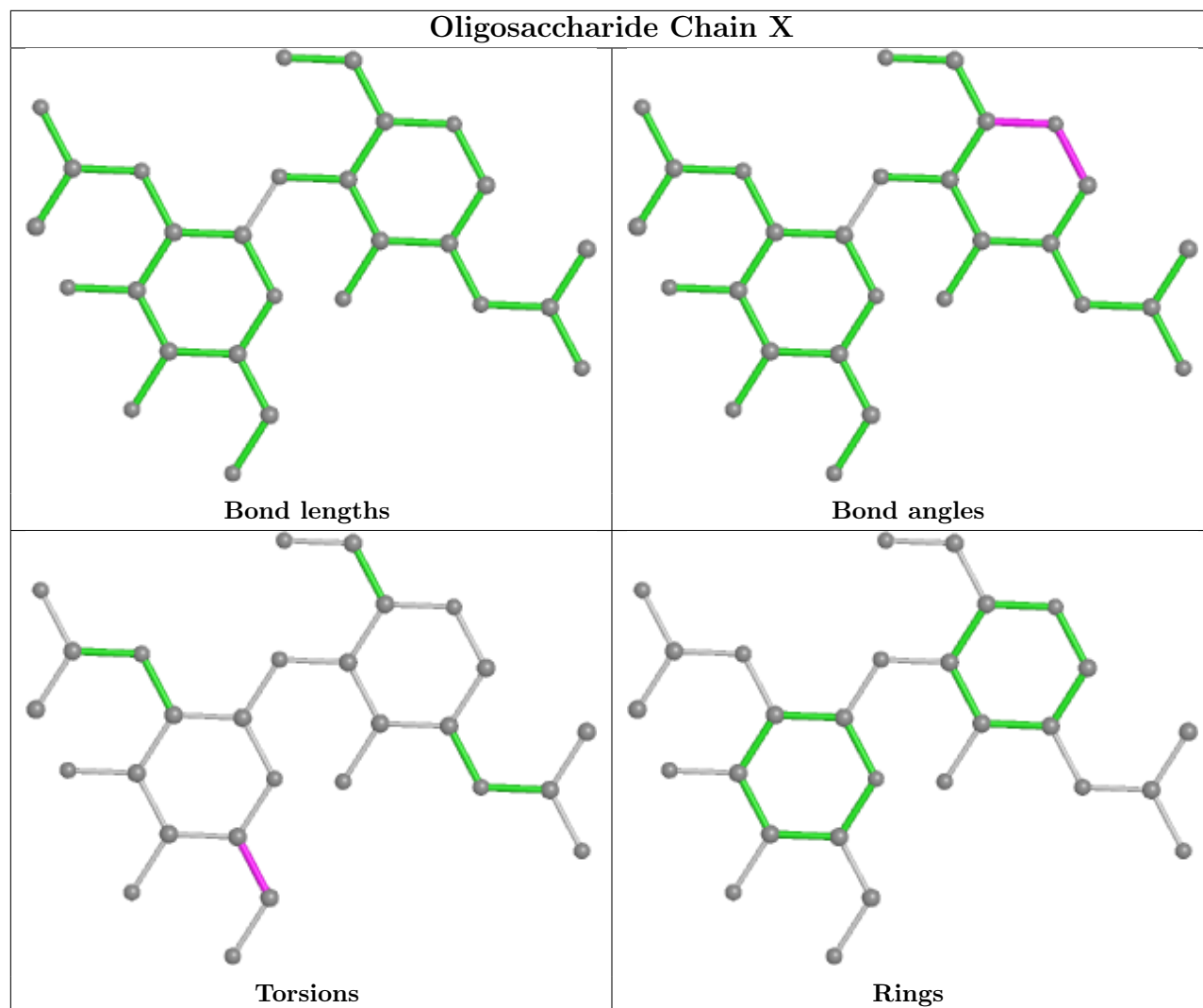


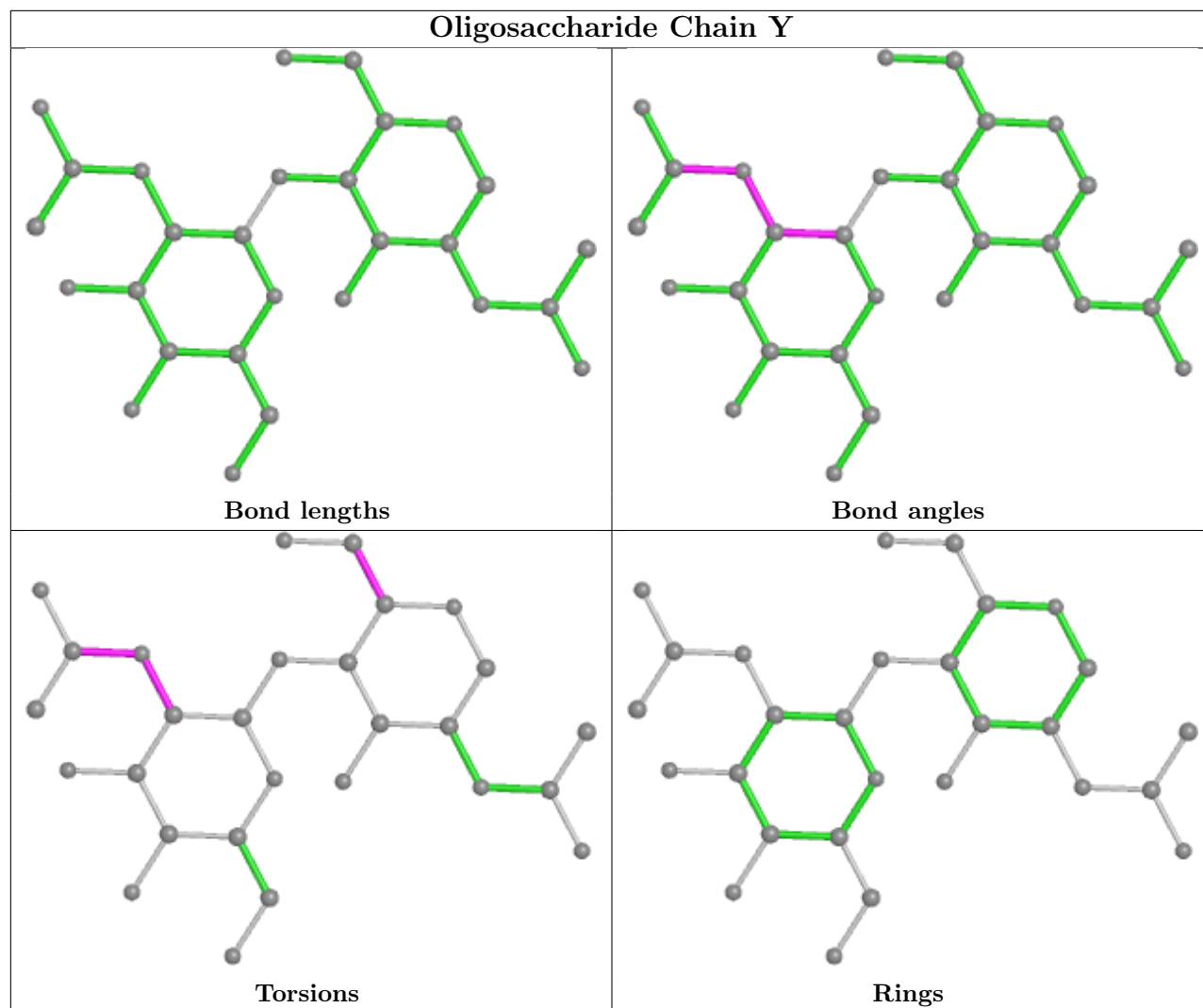


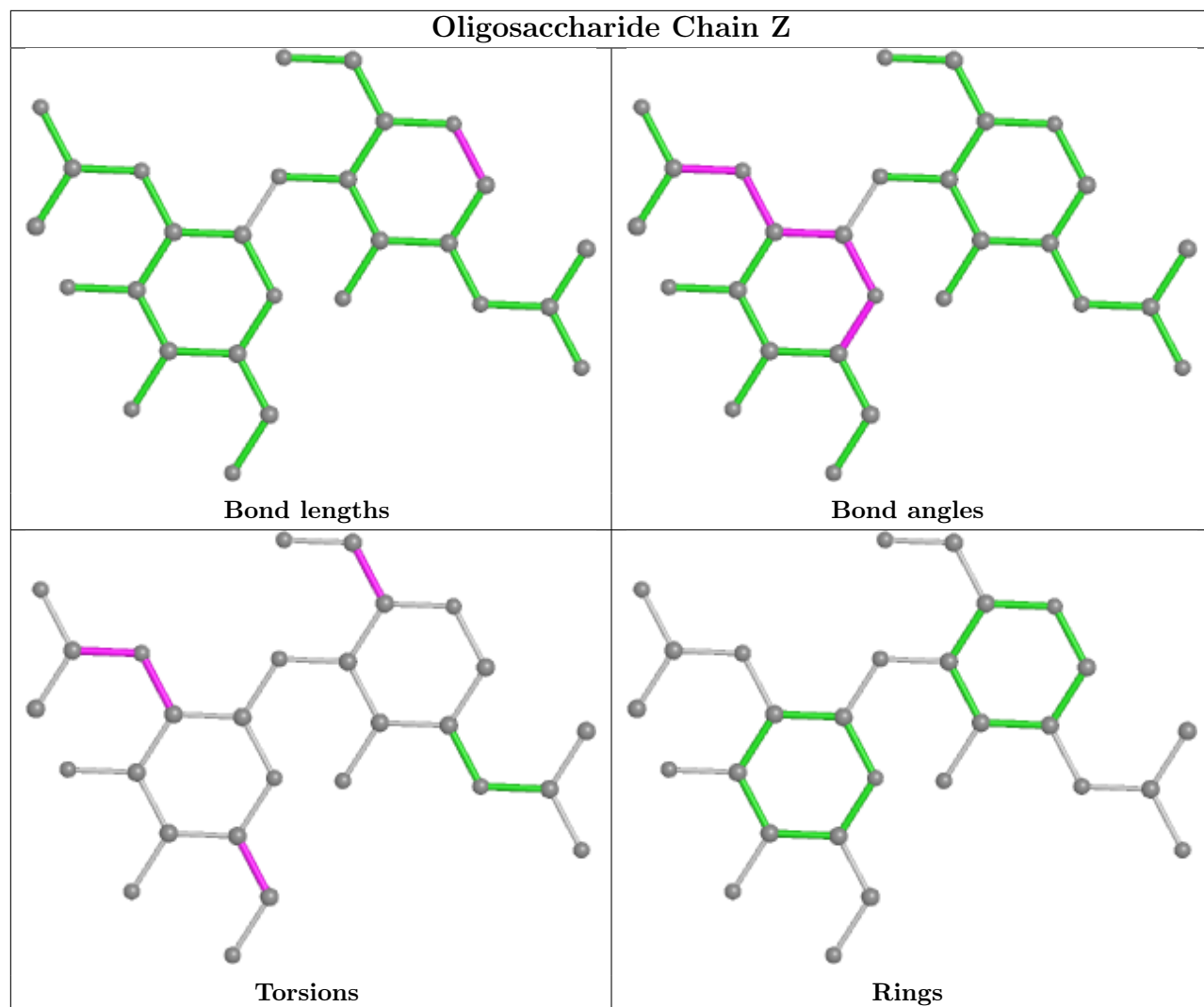


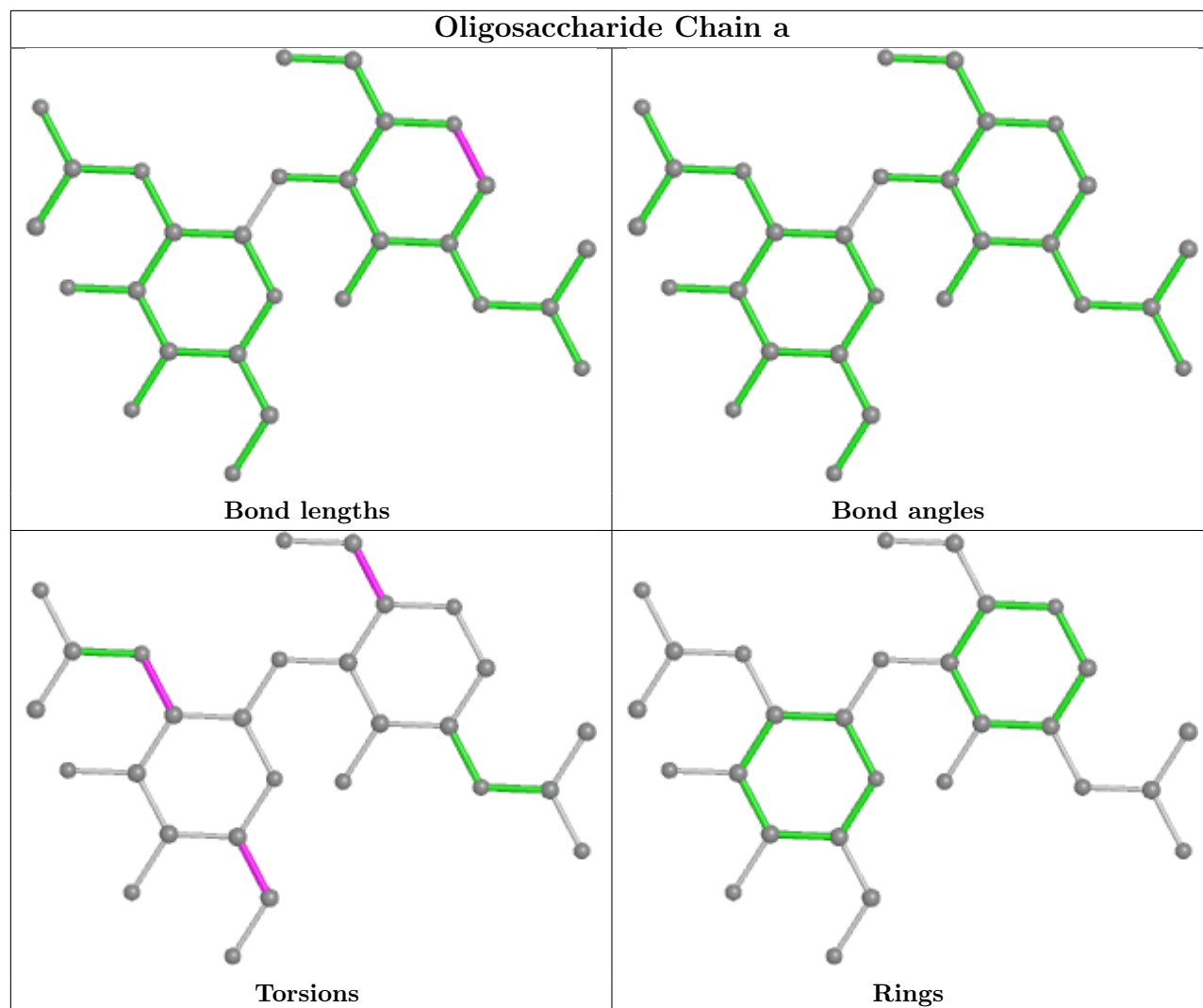


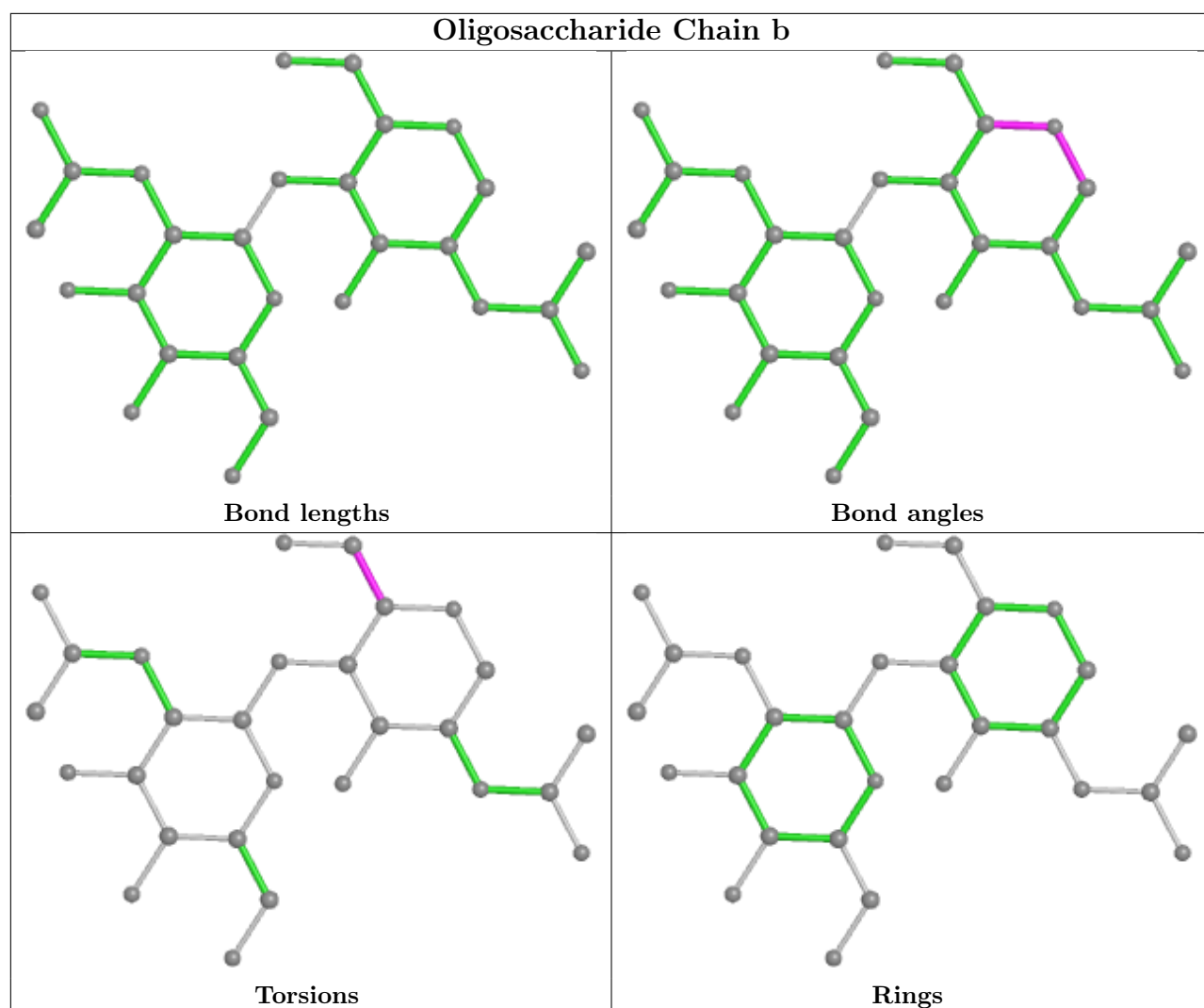


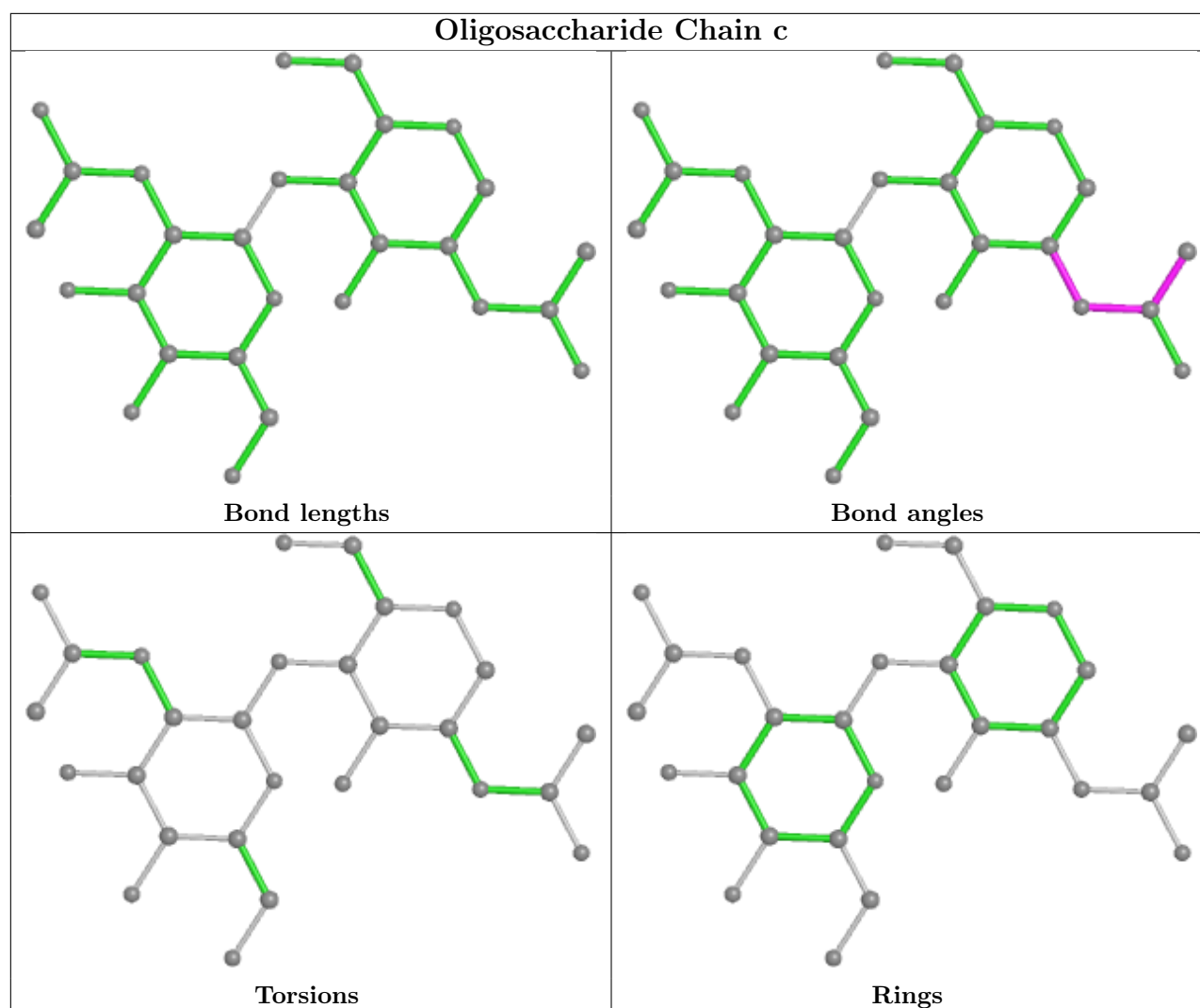












## 5.6 Ligand geometry [i](#)

26 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	1404	1	14,14,15	0.30	0	17,19,21	0.37	0
5	NAG	C	1406	1	14,14,15	0.38	0	17,19,21	0.81	1 (5%)
5	NAG	C	1402	1	14,14,15	0.34	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1401	1	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
5	NAG	C	1403	1	14,14,15	0.30	0	17,19,21	0.40	0
5	NAG	C	1404	1	14,14,15	0.33	0	17,19,21	0.59	0
5	NAG	A	1406	1	14,14,15	0.21	0	17,19,21	0.37	0
5	NAG	A	1407	1	14,14,15	0.36	0	17,19,21	0.63	0
5	NAG	B	1404	1	14,14,15	0.44	0	17,19,21	0.54	0
5	NAG	B	1408	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	C	1405	1	14,14,15	0.37	0	17,19,21	1.28	2 (11%)
5	NAG	A	1408	1	14,14,15	0.17	0	17,19,21	0.56	0
5	NAG	B	1401	1	14,14,15	0.29	0	17,19,21	0.34	0
5	NAG	B	1403	1	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	B	1409	1	14,14,15	0.49	0	17,19,21	0.36	0
5	NAG	A	1403	1	14,14,15	0.55	0	17,19,21	0.45	0
5	NAG	B	1402	1	14,14,15	0.22	0	17,19,21	0.63	0
5	NAG	A	1402	1	14,14,15	0.46	0	17,19,21	0.57	0
5	NAG	C	1407	1	14,14,15	0.42	0	17,19,21	0.74	1 (5%)
5	NAG	C	1408	1	14,14,15	0.33	0	17,19,21	0.41	0
5	NAG	B	1407	1	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	C	1401	1	14,14,15	0.29	0	17,19,21	0.55	0
5	NAG	B	1406	1	14,14,15	0.29	0	17,19,21	0.39	0
5	NAG	C	1409	1	14,14,15	0.19	0	17,19,21	0.40	0
5	NAG	B	1405	1	14,14,15	0.56	0	17,19,21	1.26	1 (5%)
5	NAG	A	1405	1	14,14,15	0.36	0	17,19,21	1.29	2 (11%)

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	1404	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	2/6/23/26	0/1/1/1

Continued on next page...



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1405	NAG	C2-N2-C7	4.31	129.05	122.90
5	A	1405	NAG	C2-N2-C7	4.29	129.02	122.90
5	C	1405	NAG	C2-N2-C7	4.15	128.81	122.90
5	A	1401	NAG	C1-O5-C5	2.88	116.09	112.19
5	C	1406	NAG	C1-O5-C5	2.57	115.67	112.19

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

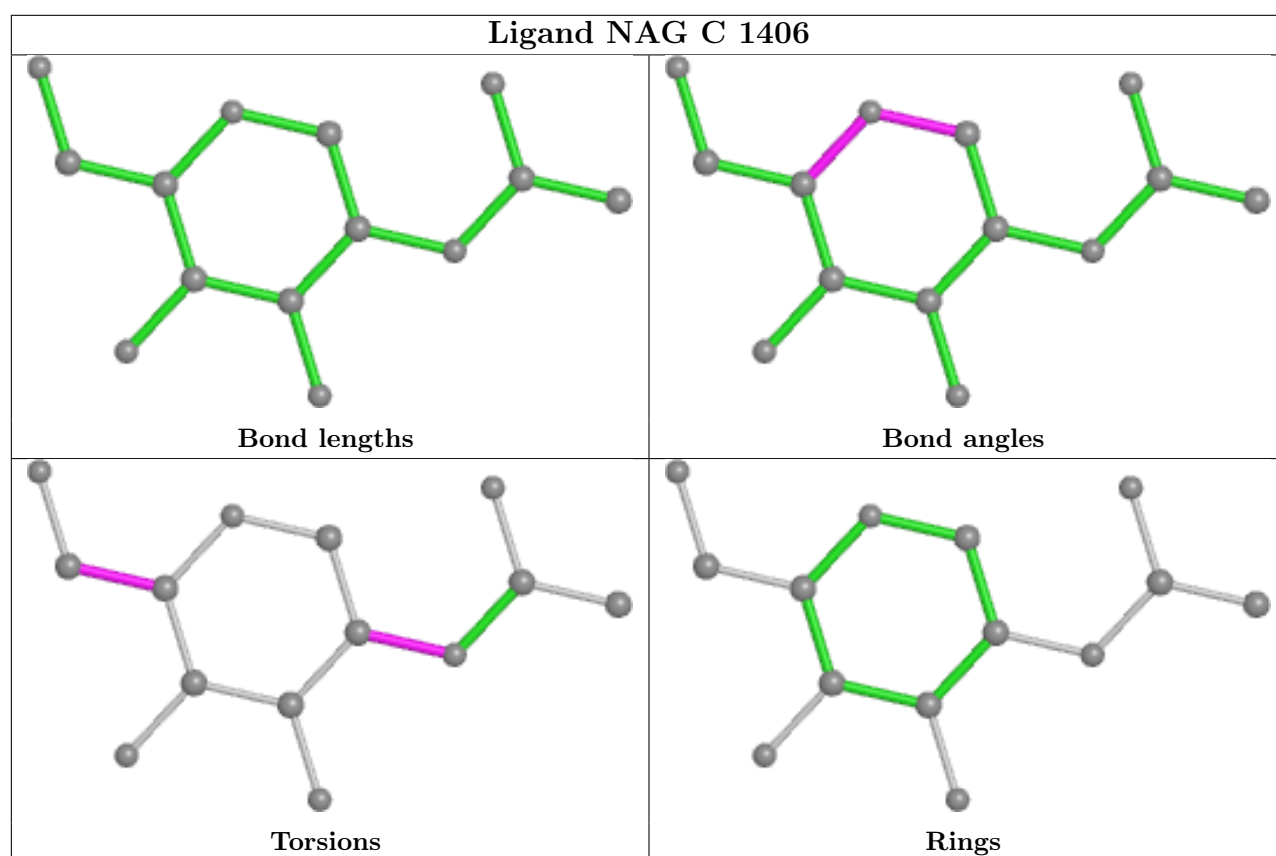
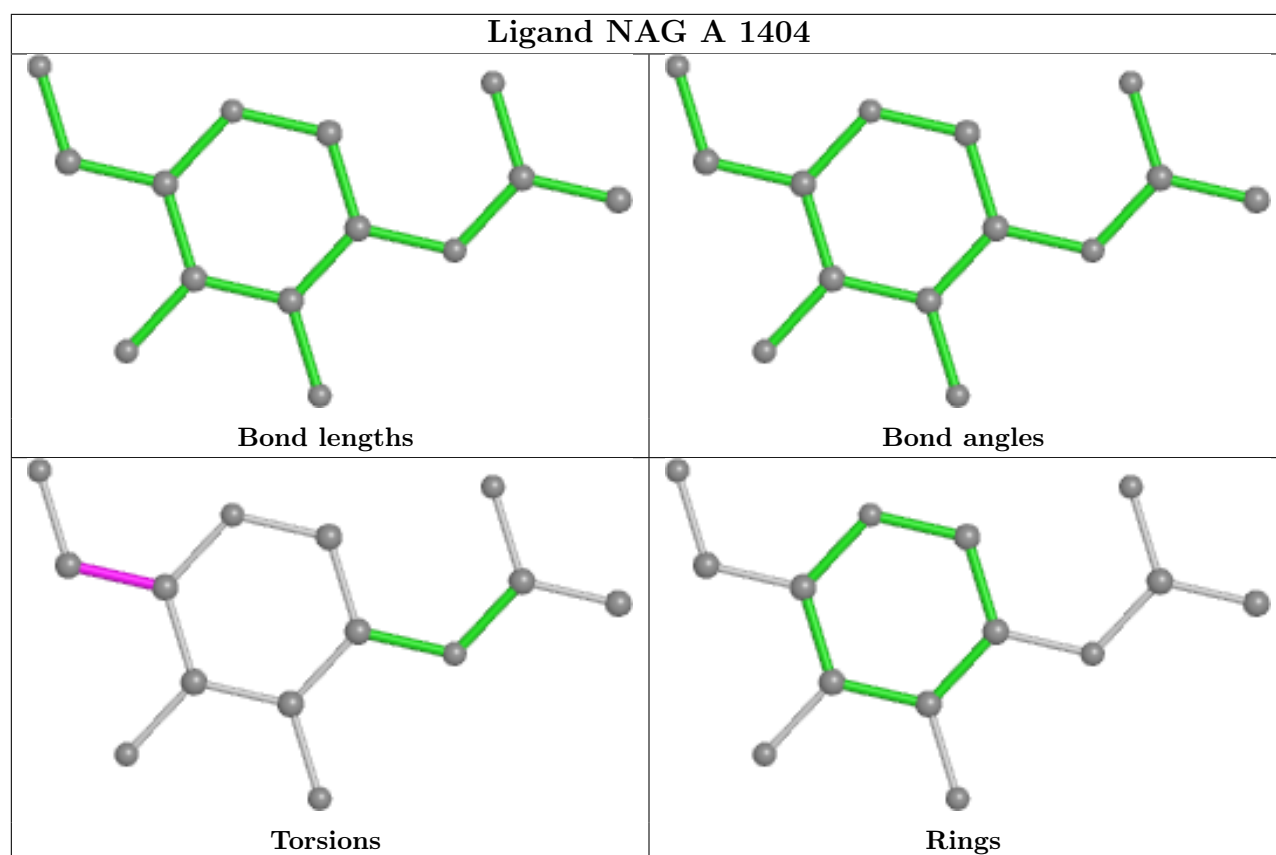
Mol	Chain	Res	Type	Atoms
5	C	1408	NAG	O5-C5-C6-O6
5	C	1401	NAG	O5-C5-C6-O6
5	A	1408	NAG	O5-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	B	1406	NAG	O5-C5-C6-O6

There are no ring outliers.

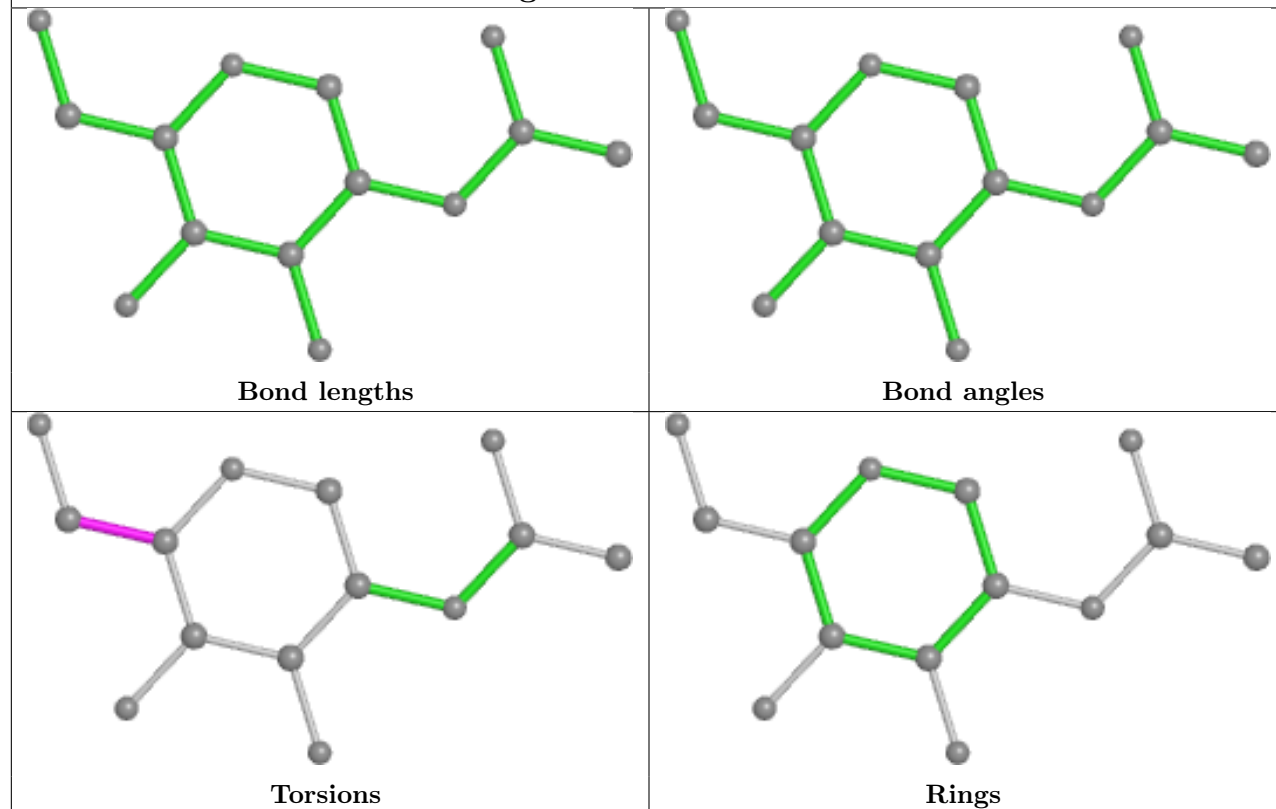
8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1402	NAG	1	0
5	C	1403	NAG	2	0
5	C	1405	NAG	2	0
5	B	1402	NAG	3	0
5	A	1402	NAG	1	0
5	C	1407	NAG	1	0
5	B	1405	NAG	1	0
5	A	1405	NAG	1	0

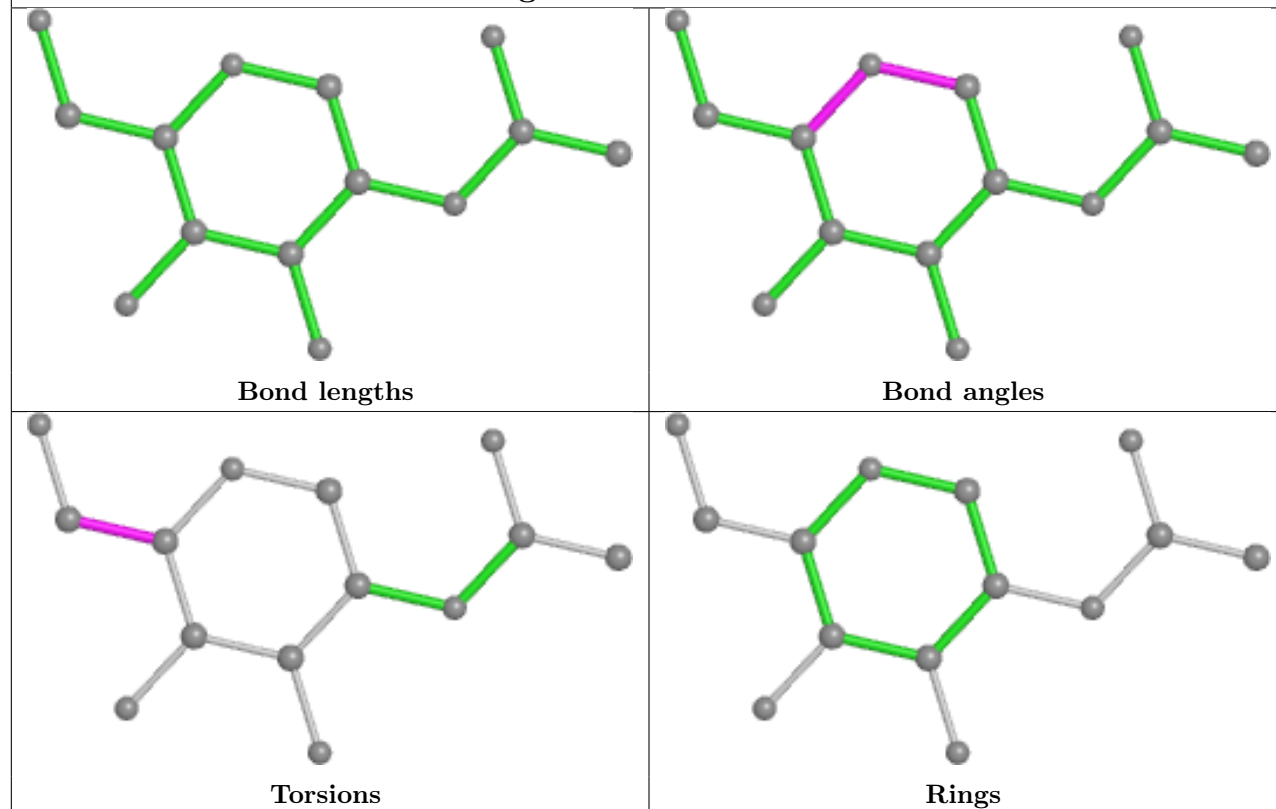
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



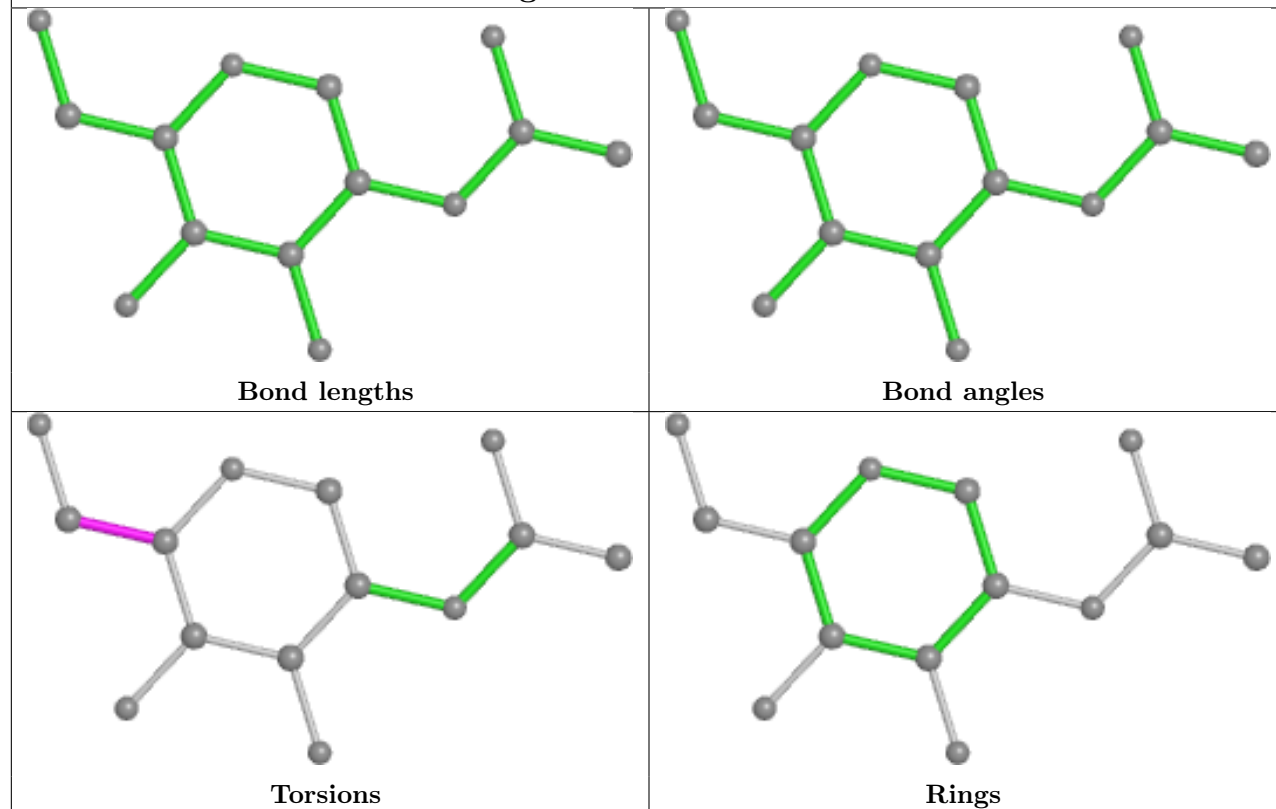
## Ligand NAG C 1402



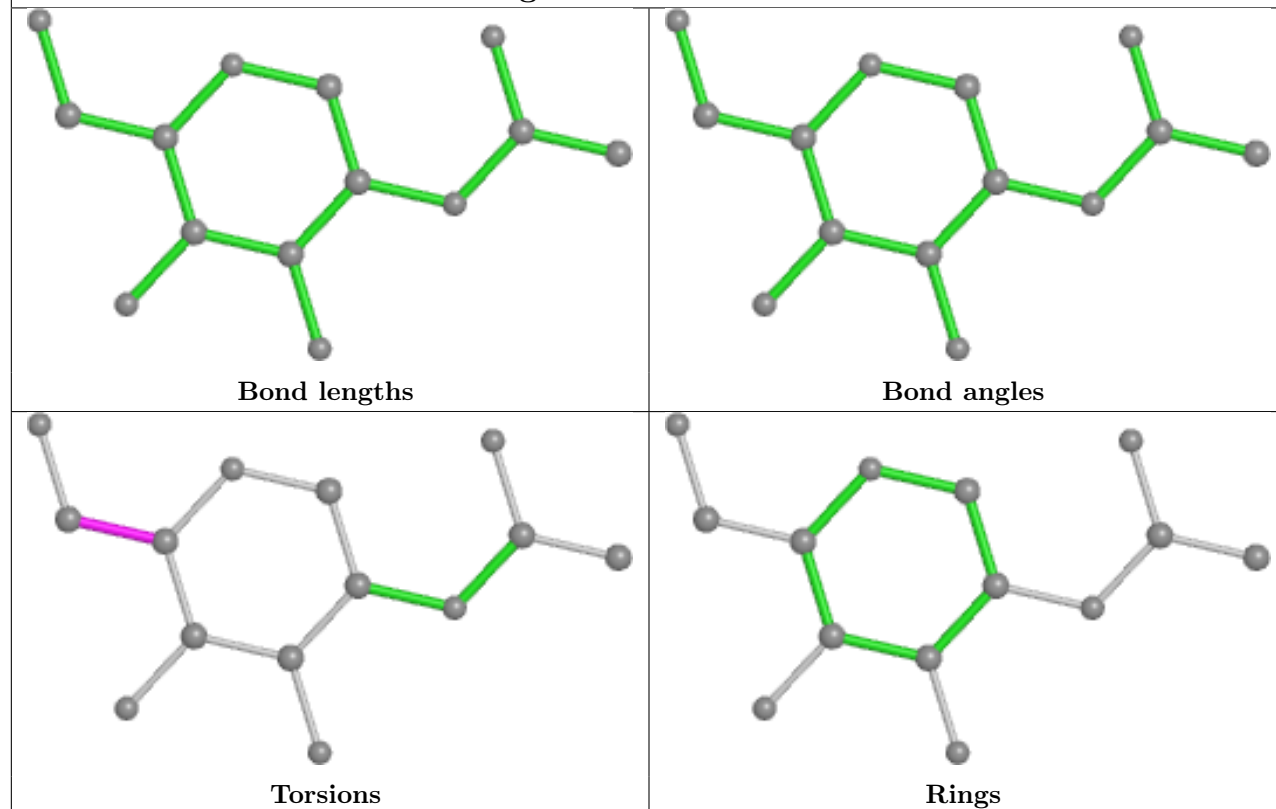
## Ligand NAG A 1401

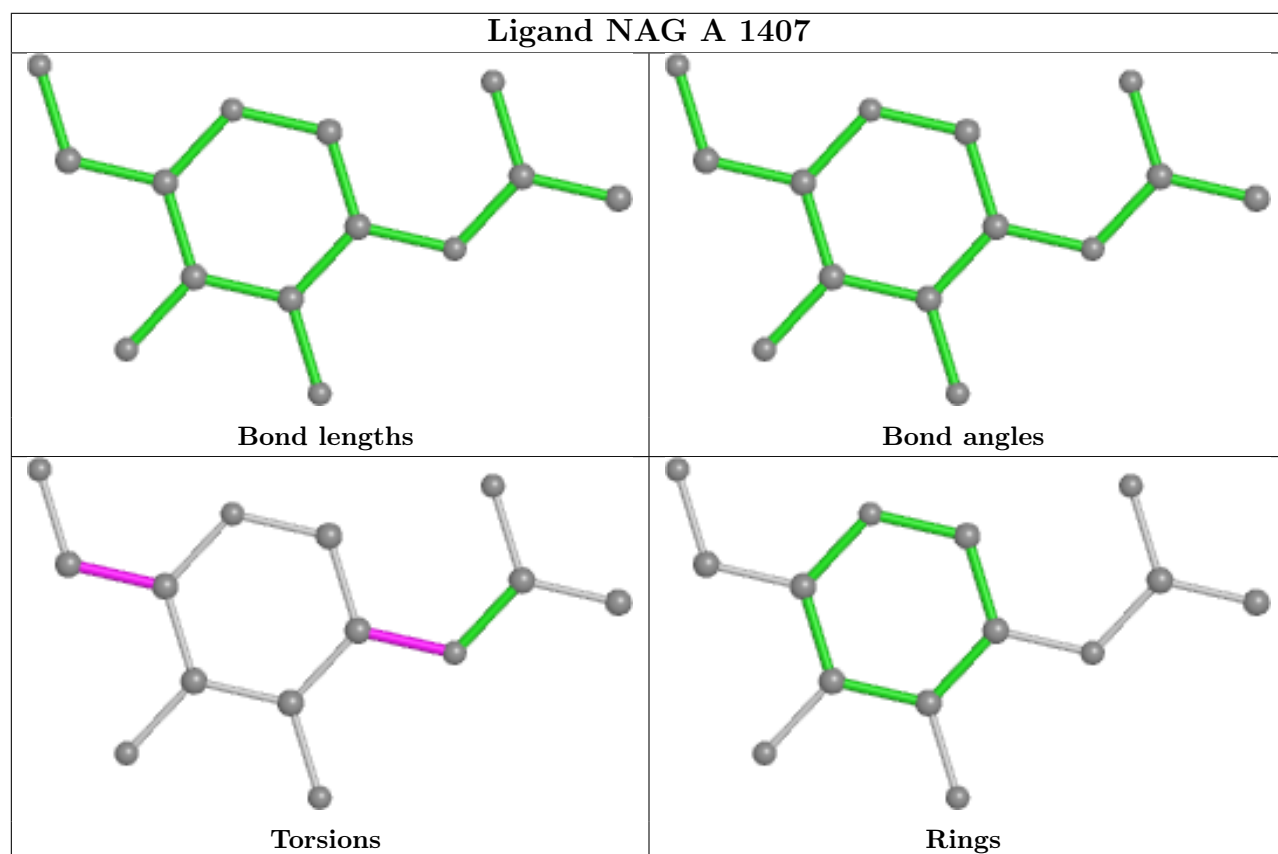
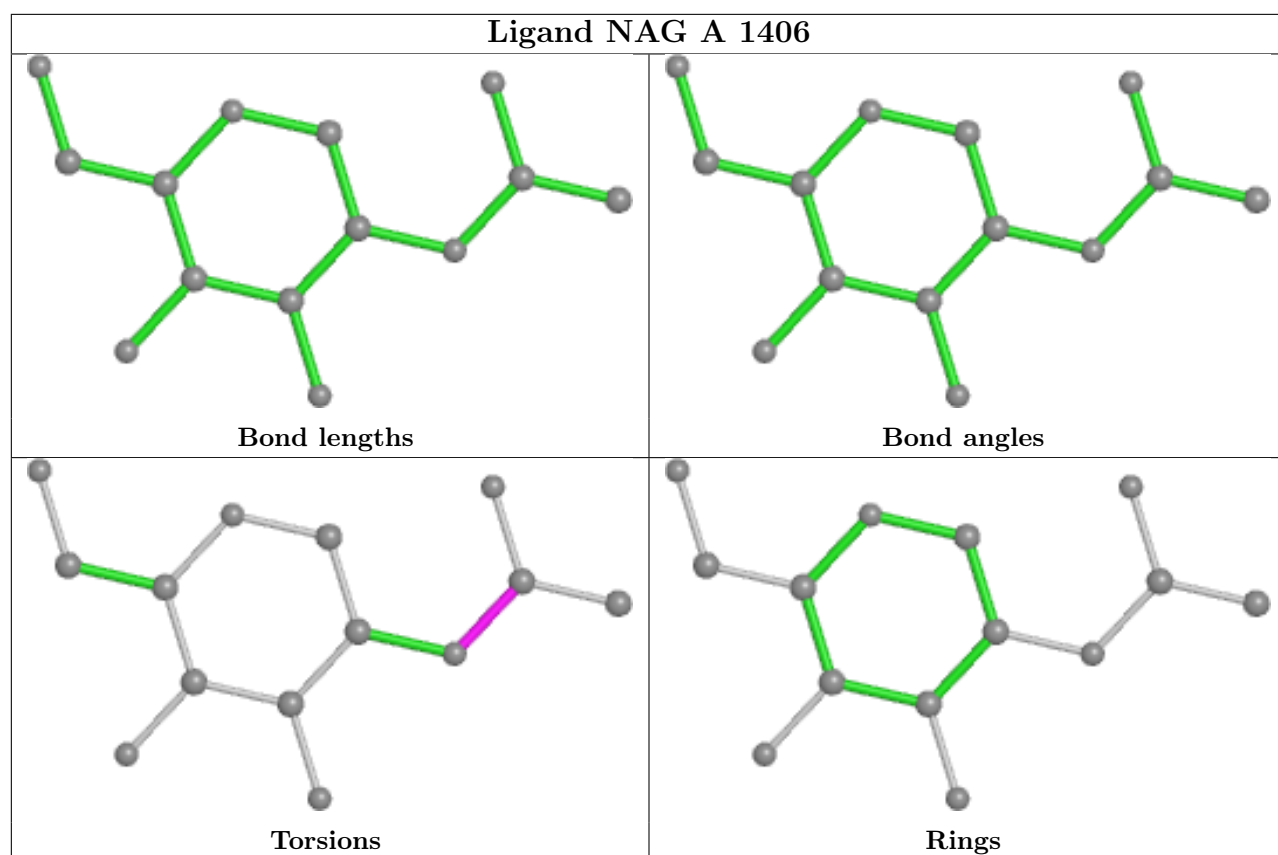


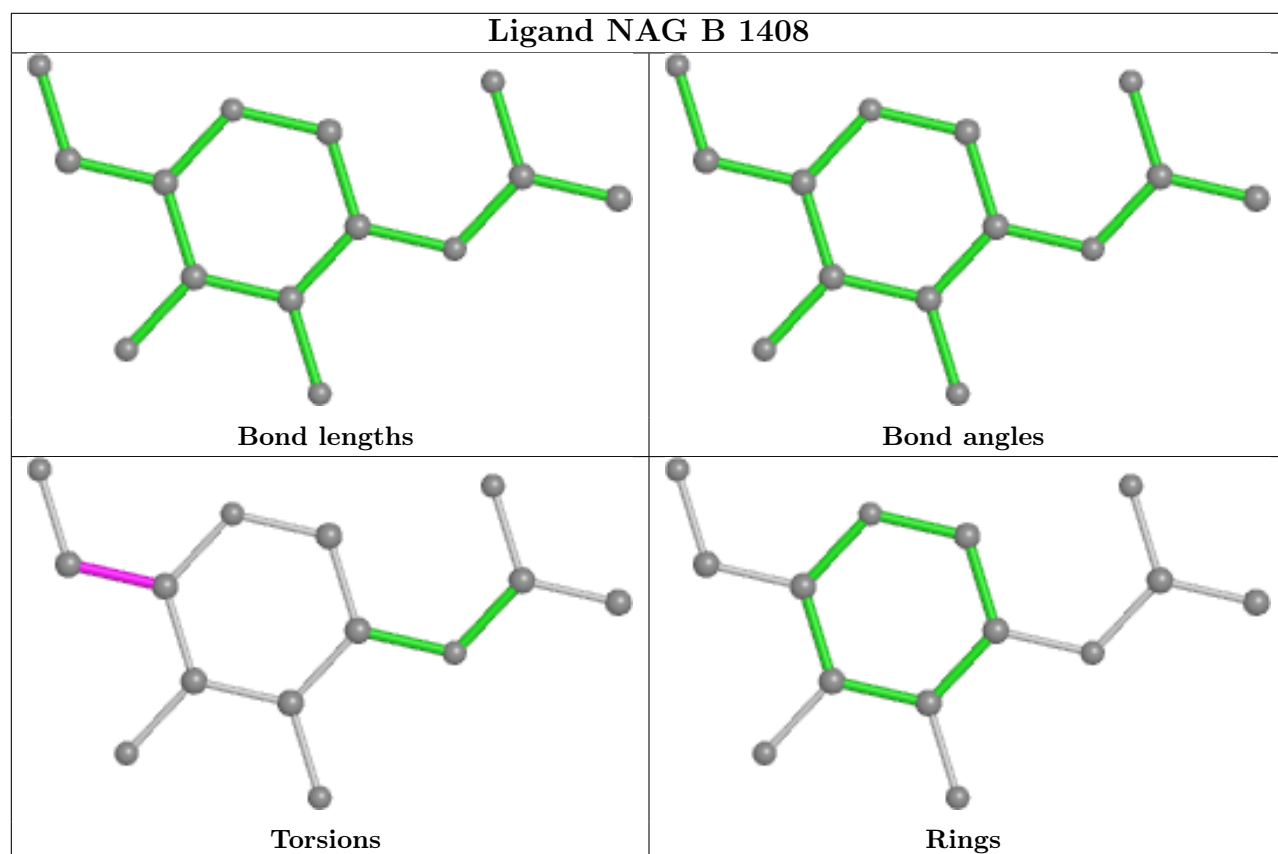
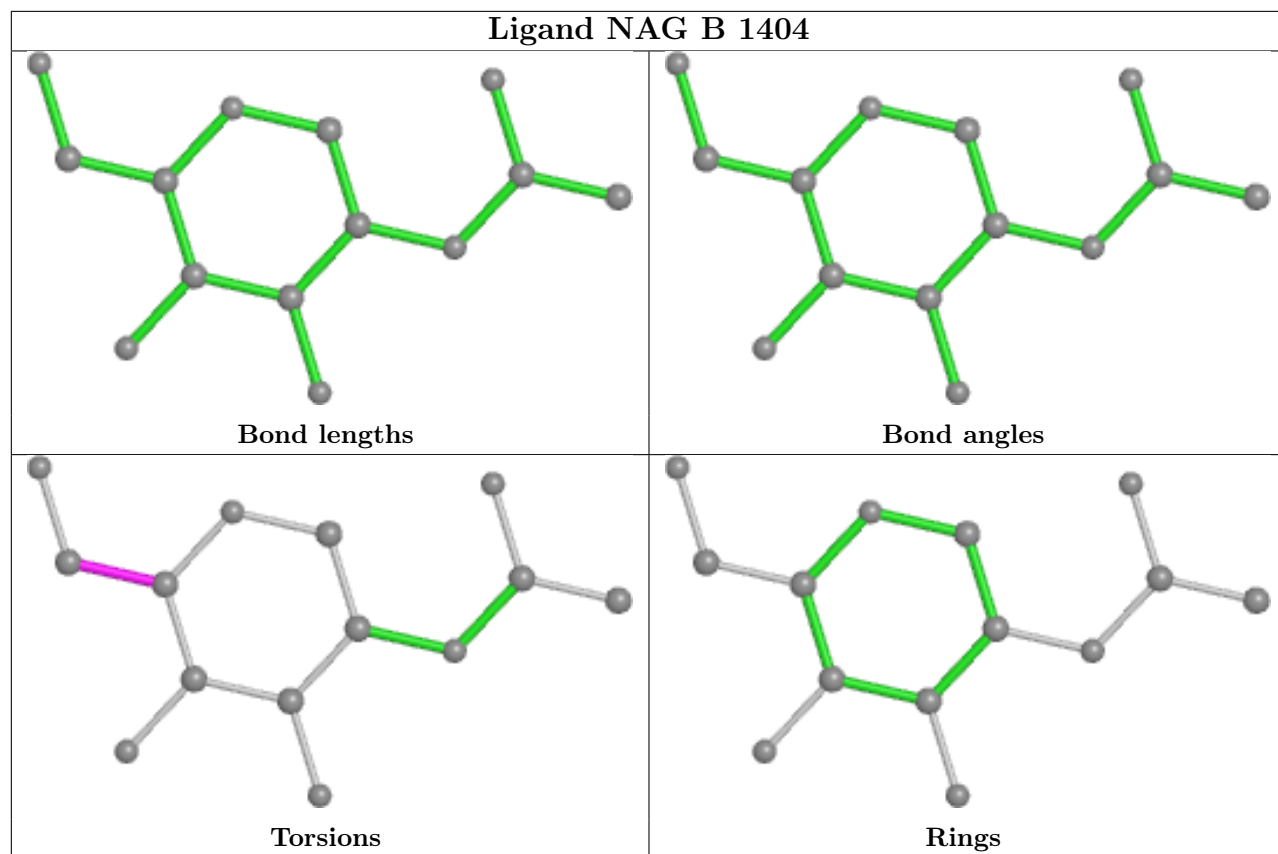
## Ligand NAG C 1403



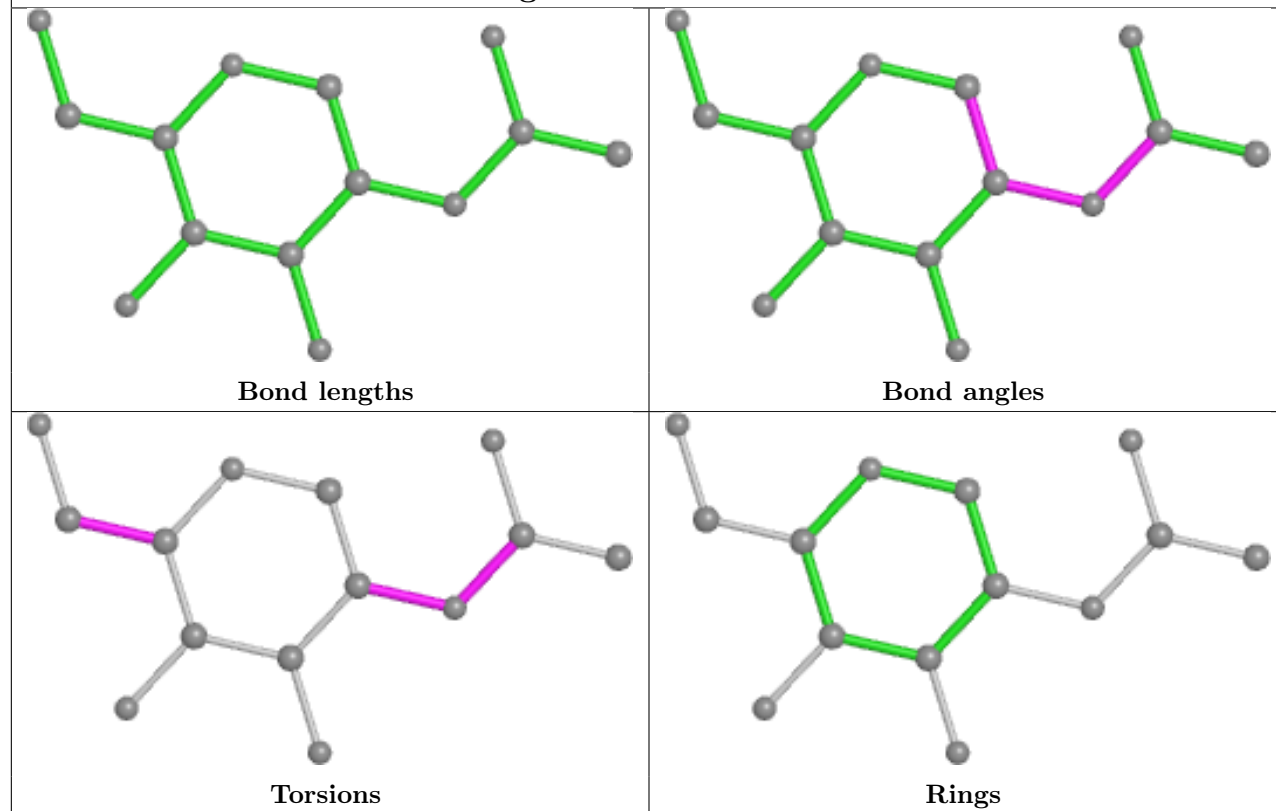
## Ligand NAG C 1404



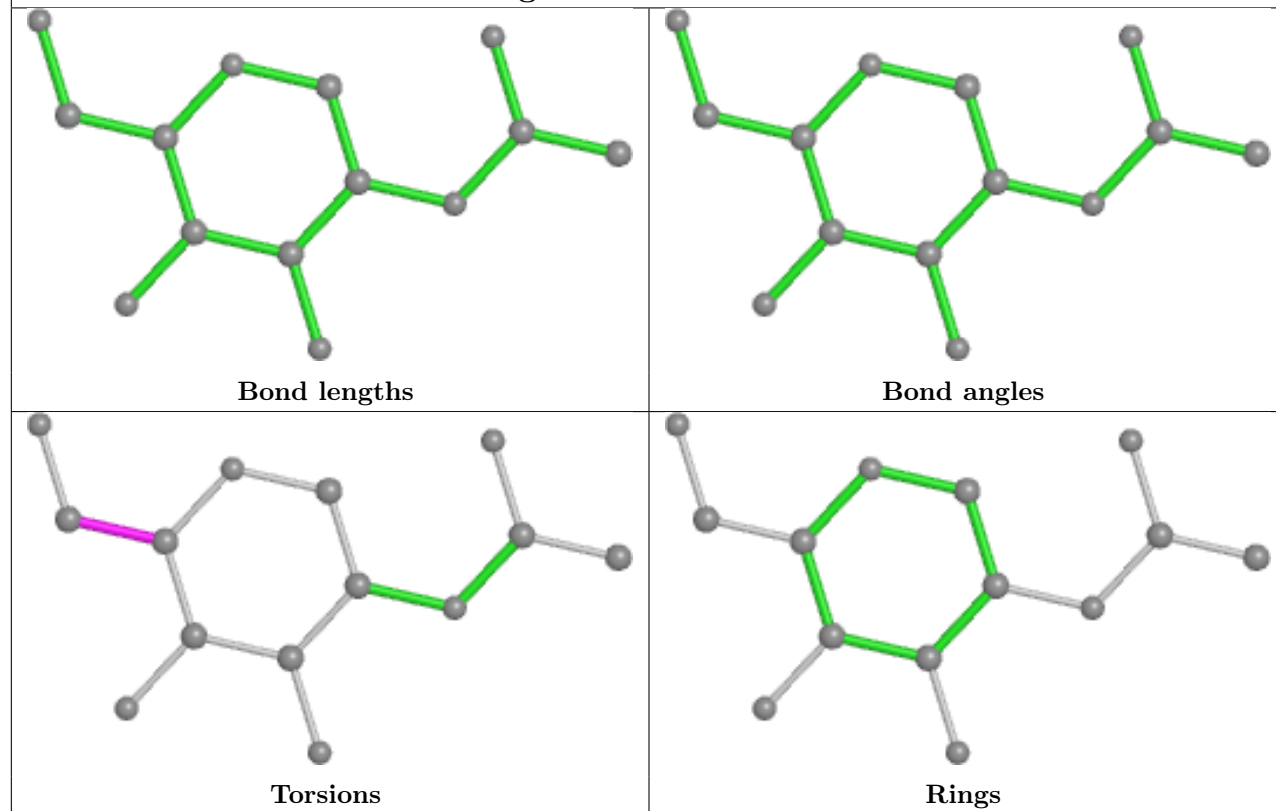




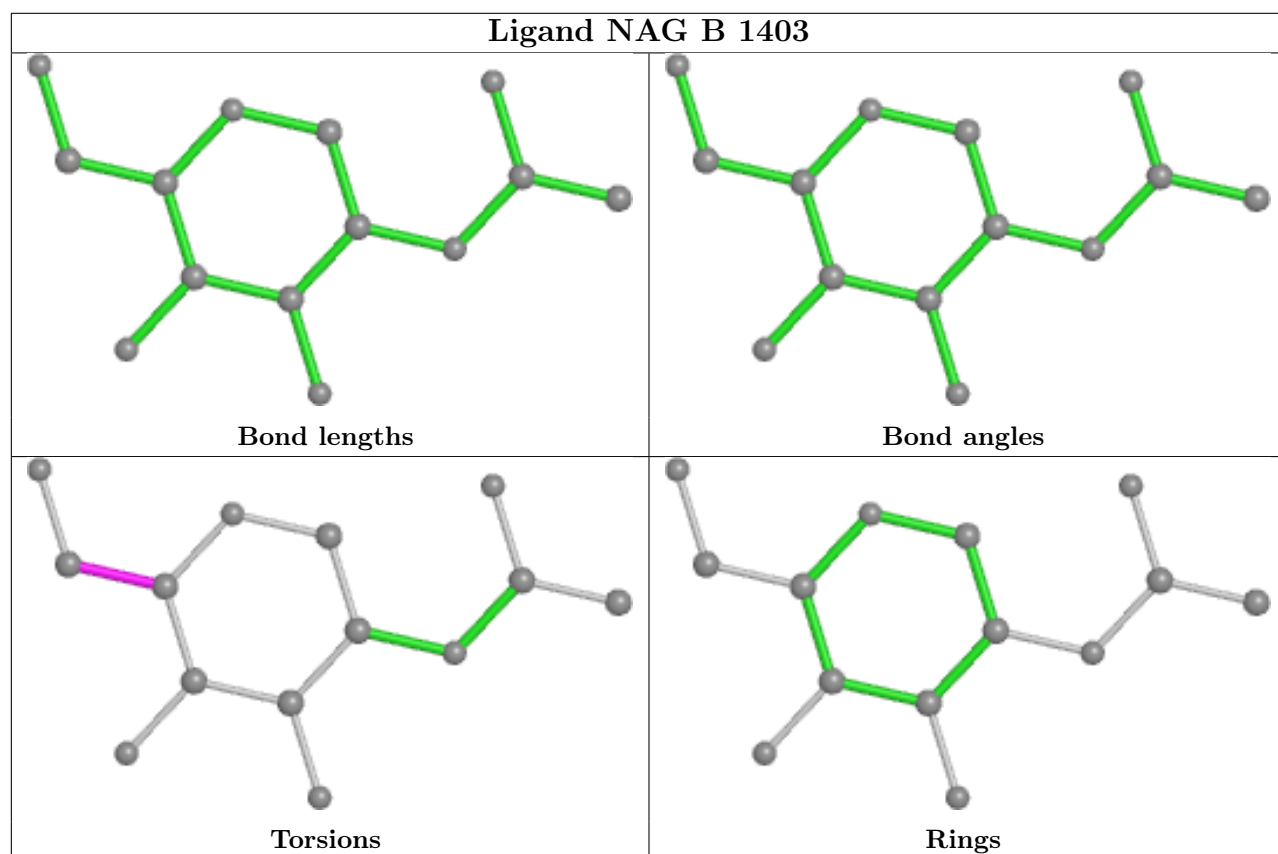
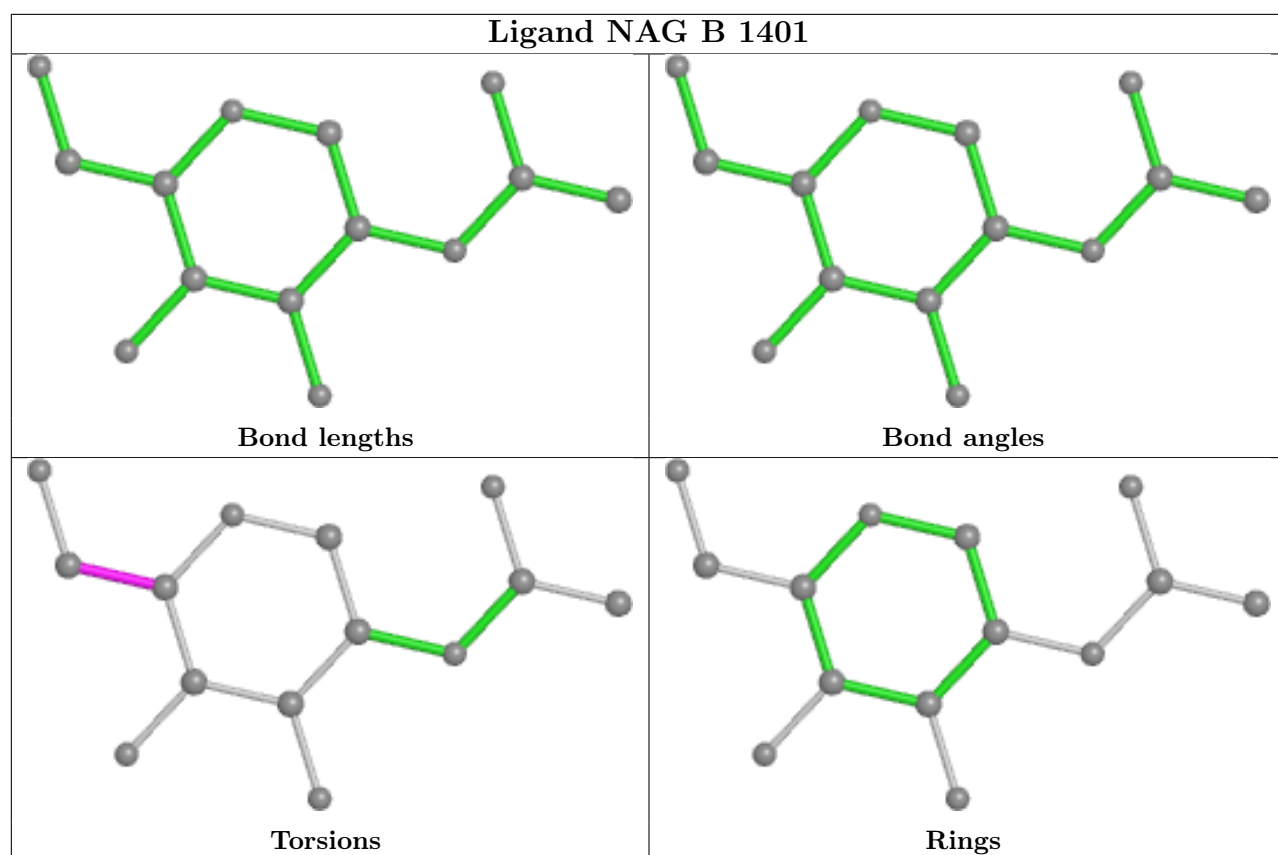
## Ligand NAG C 1405



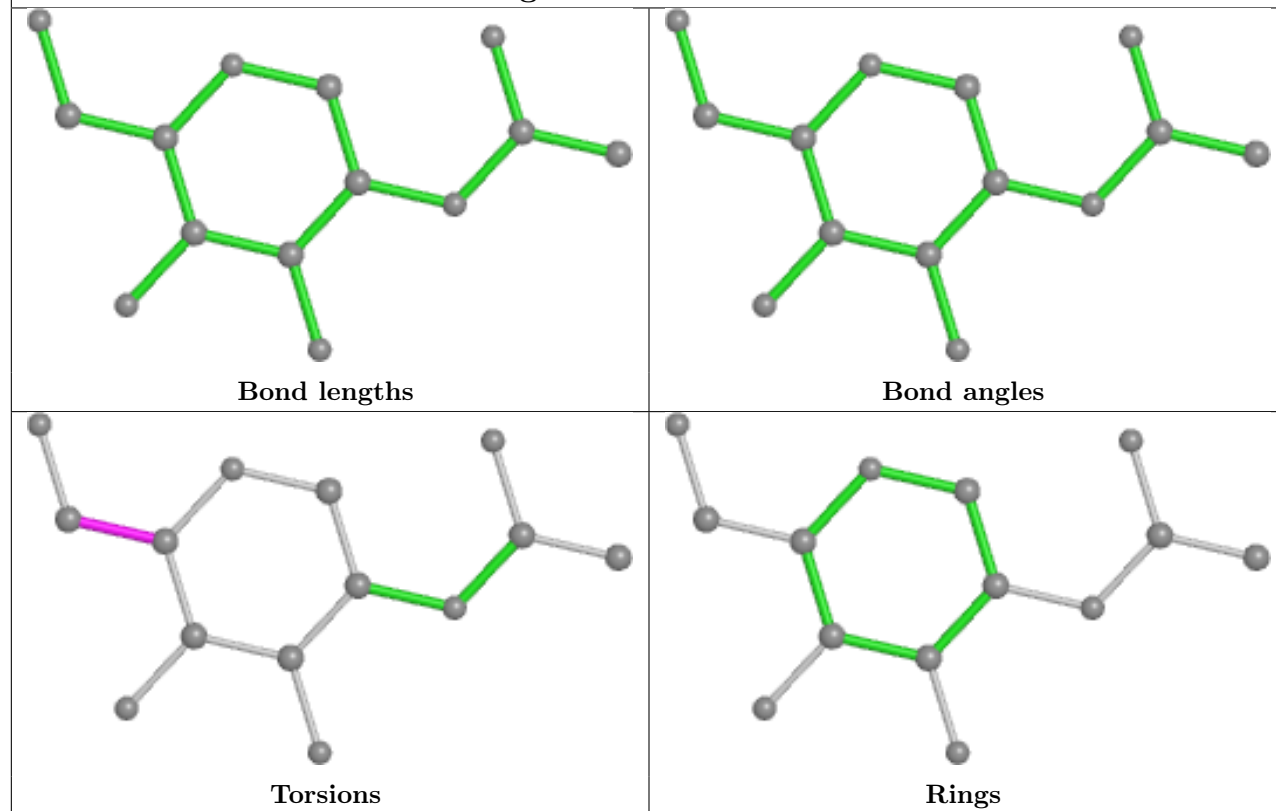
## Ligand NAG A 1408



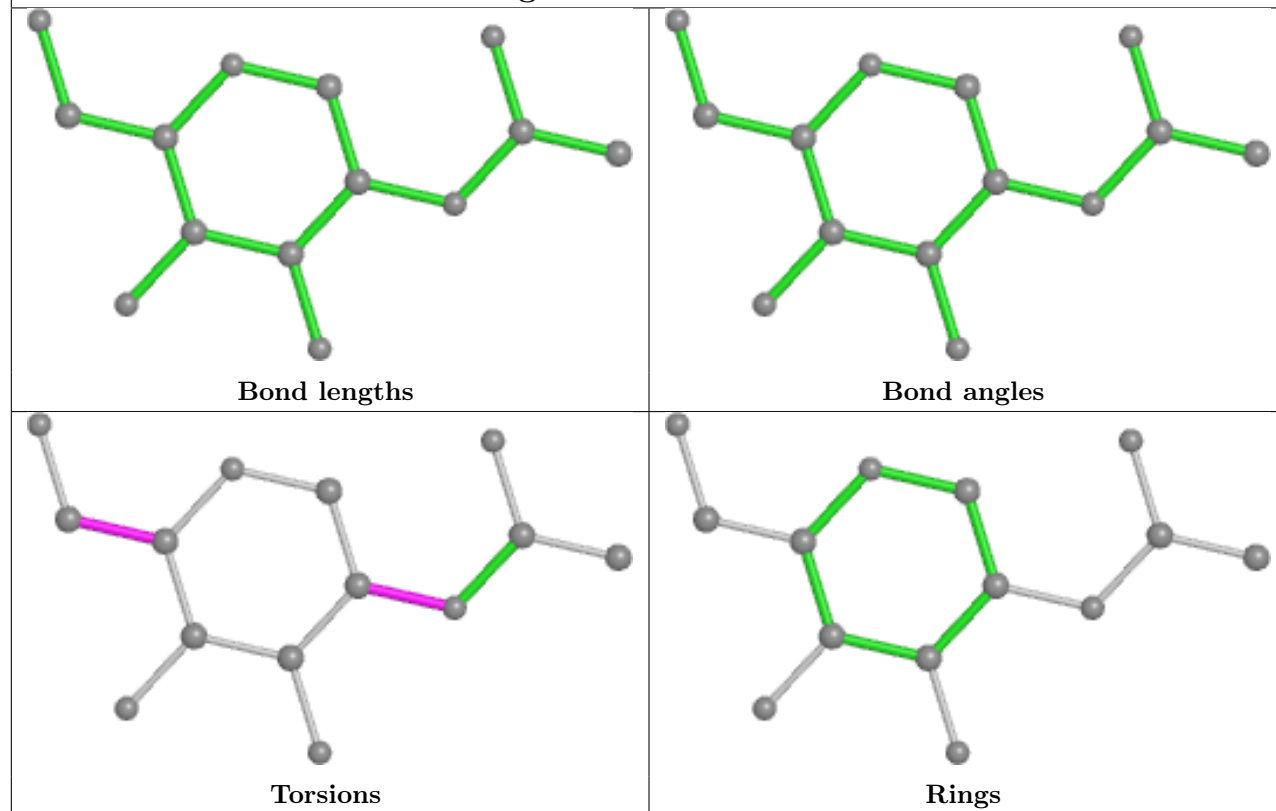


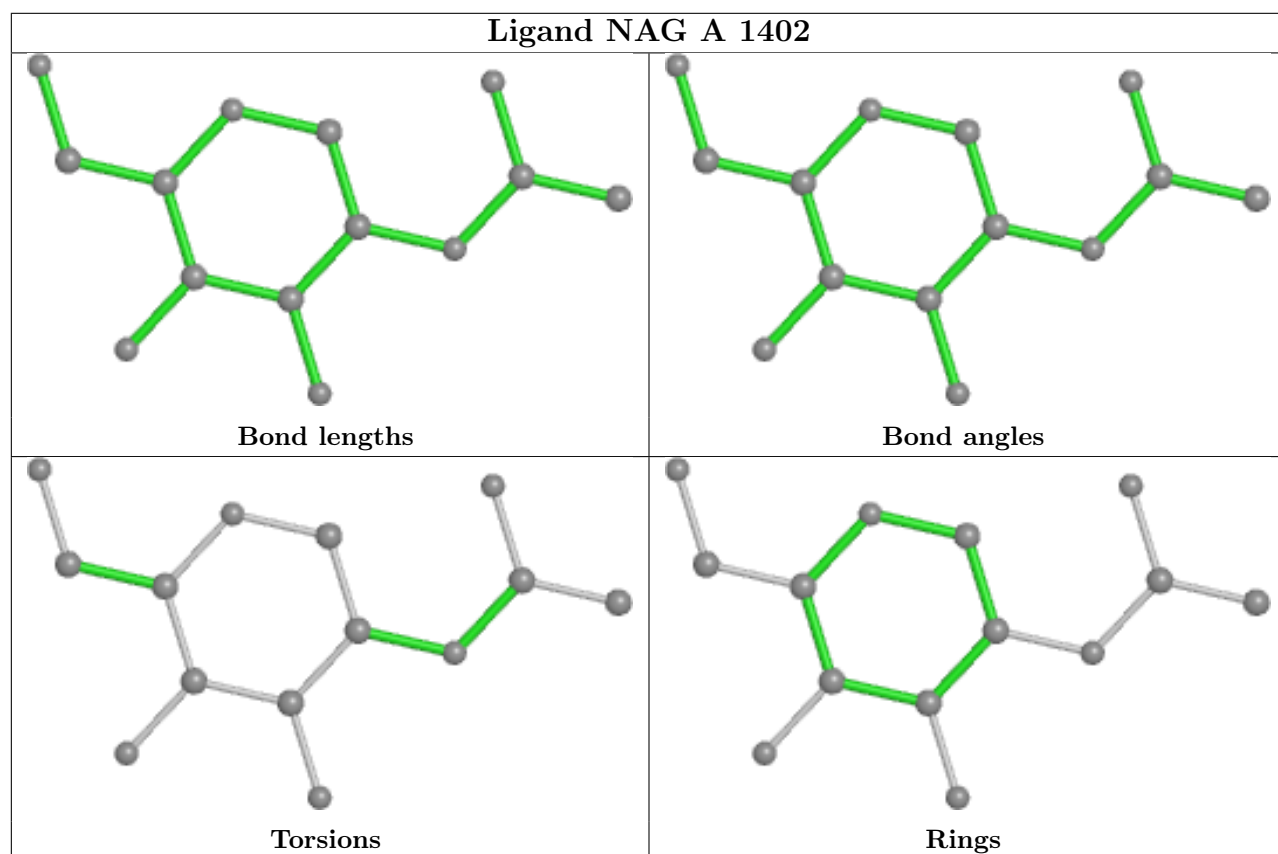
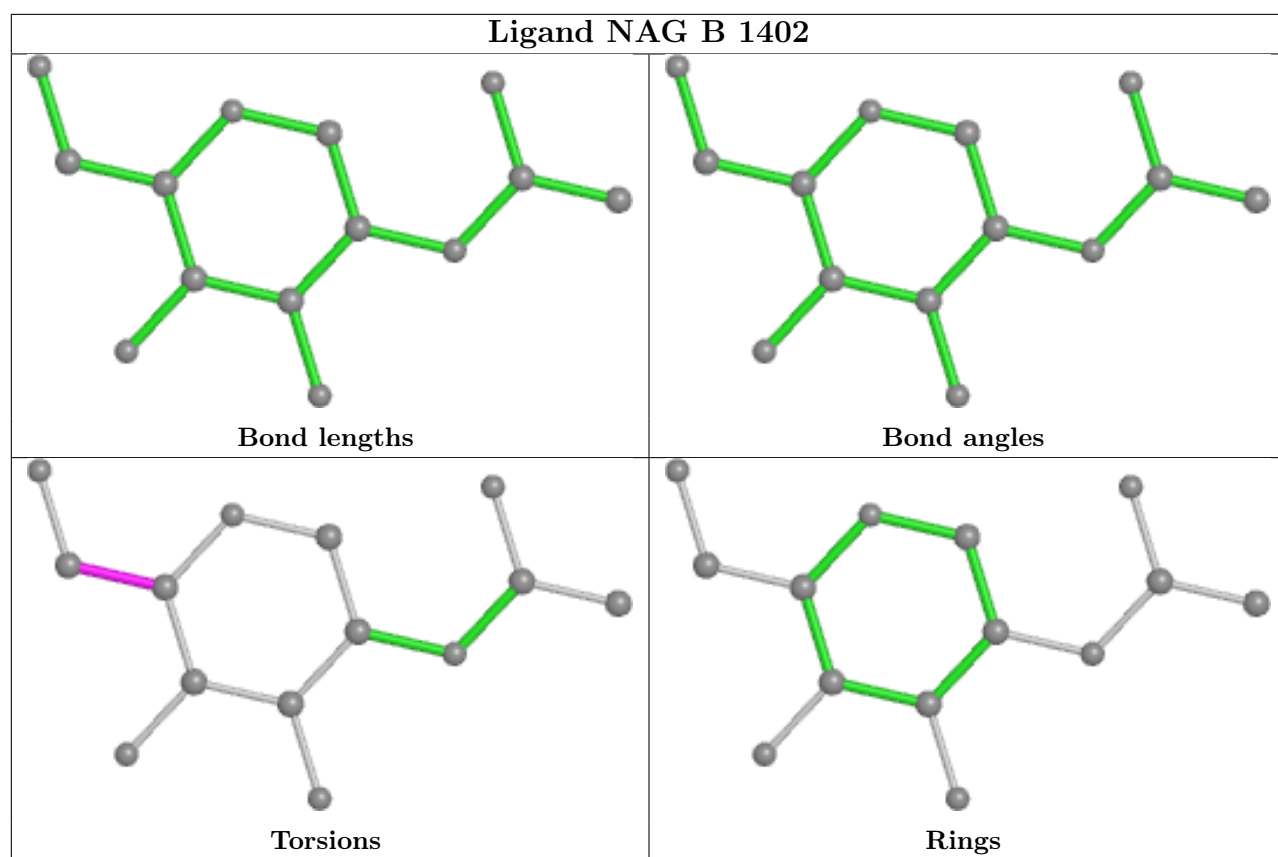


## Ligand NAG B 1409

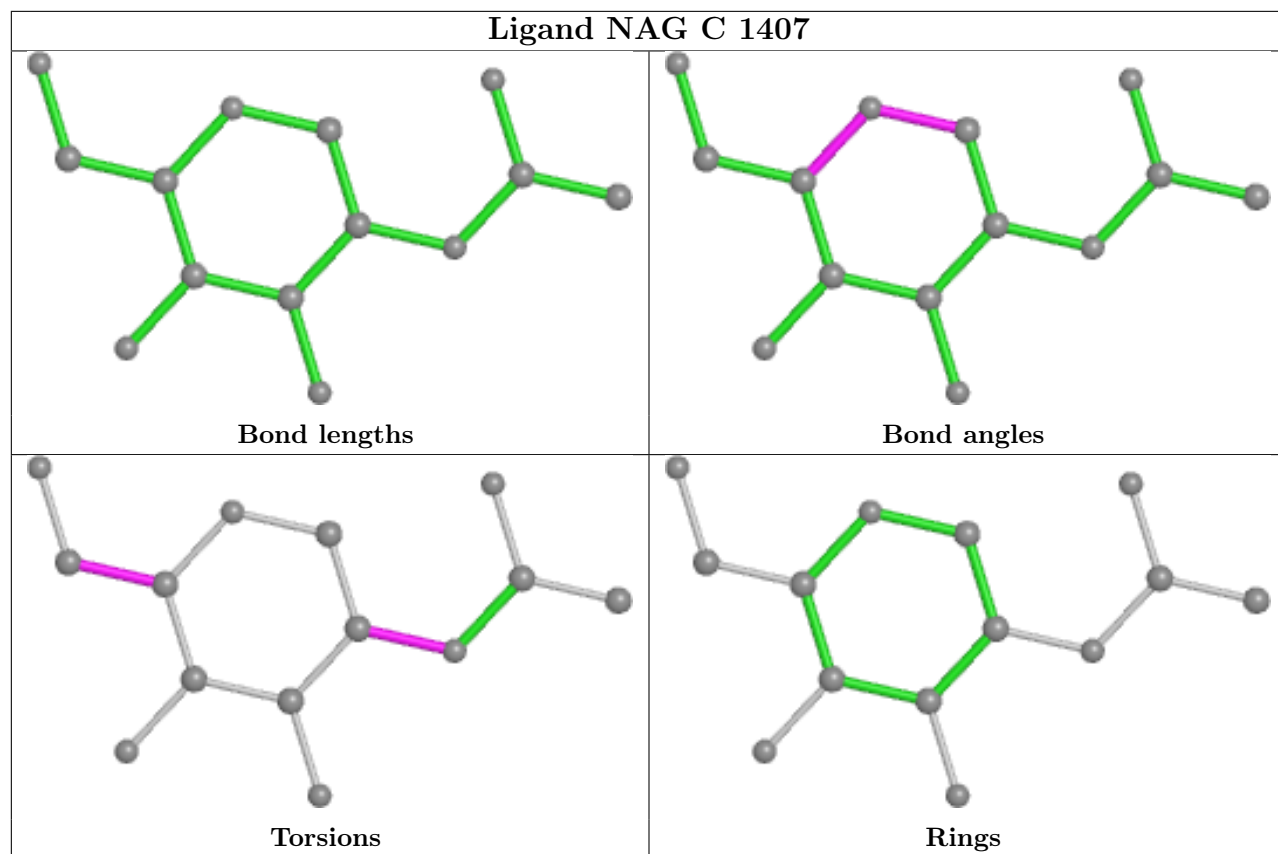


## Ligand NAG A 1403

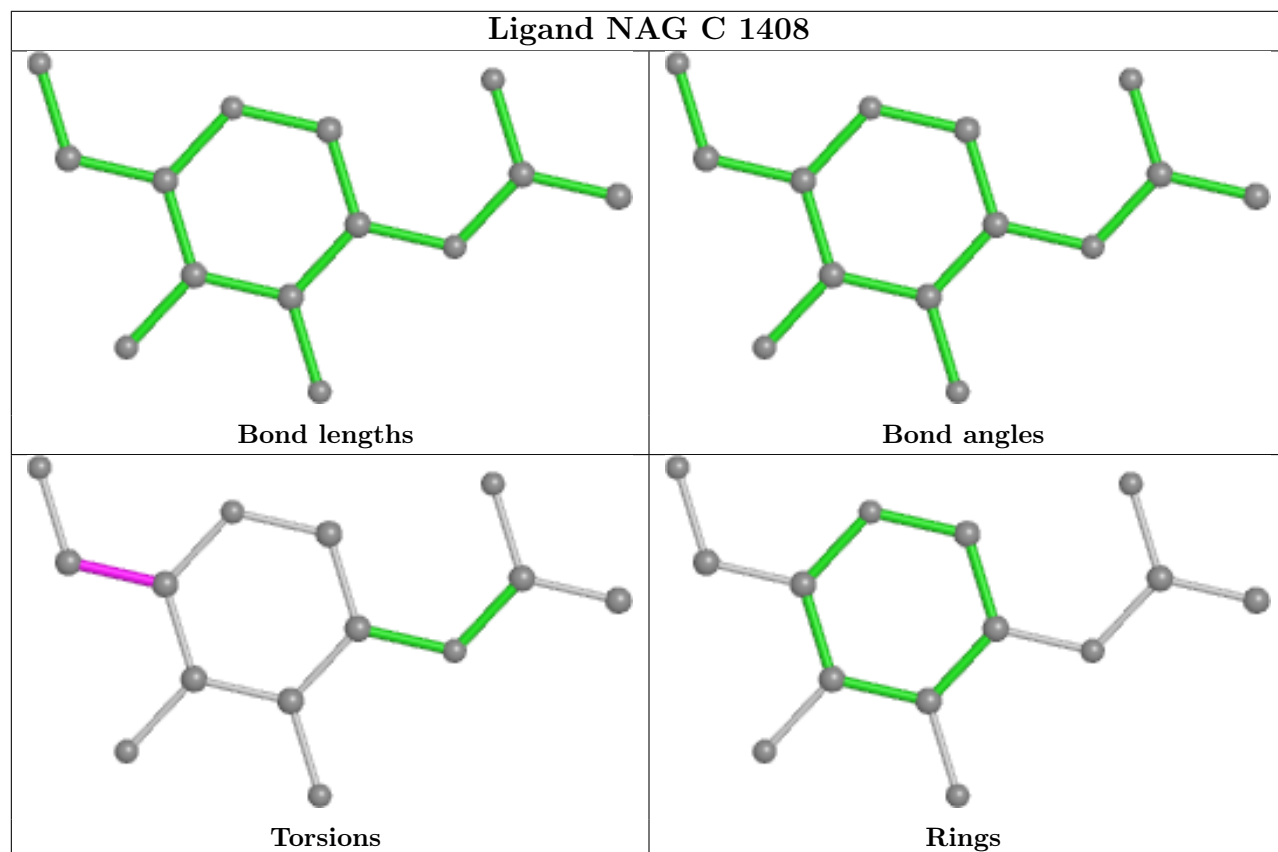


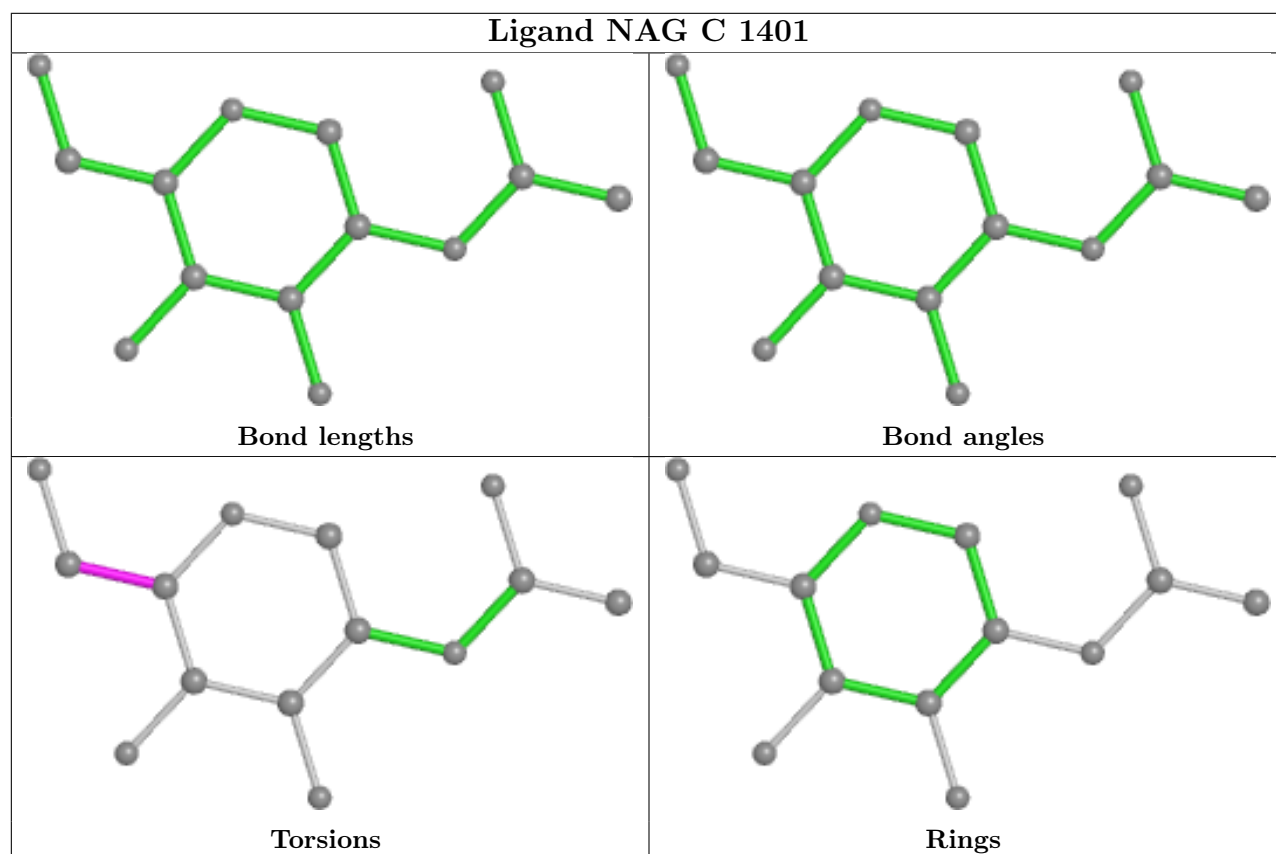
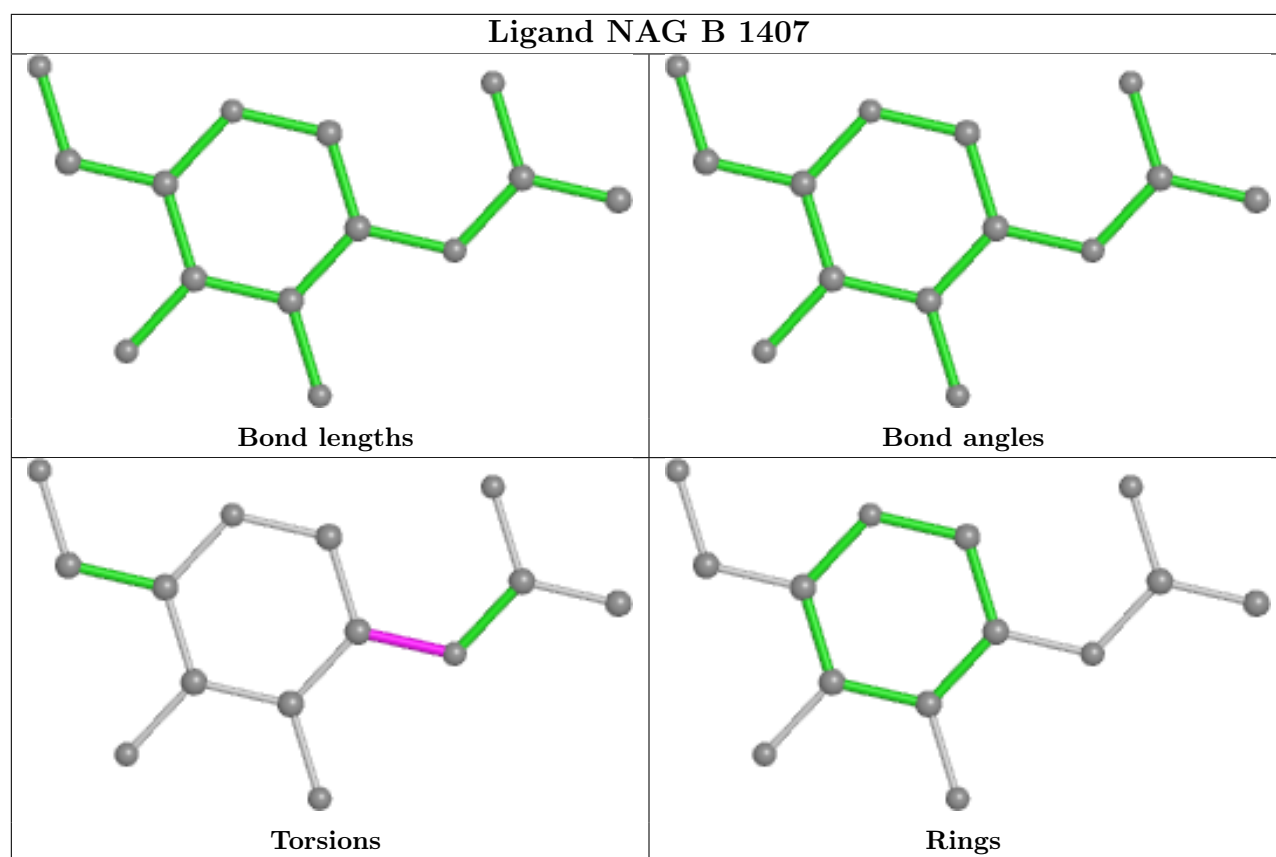


## Ligand NAG C 1407

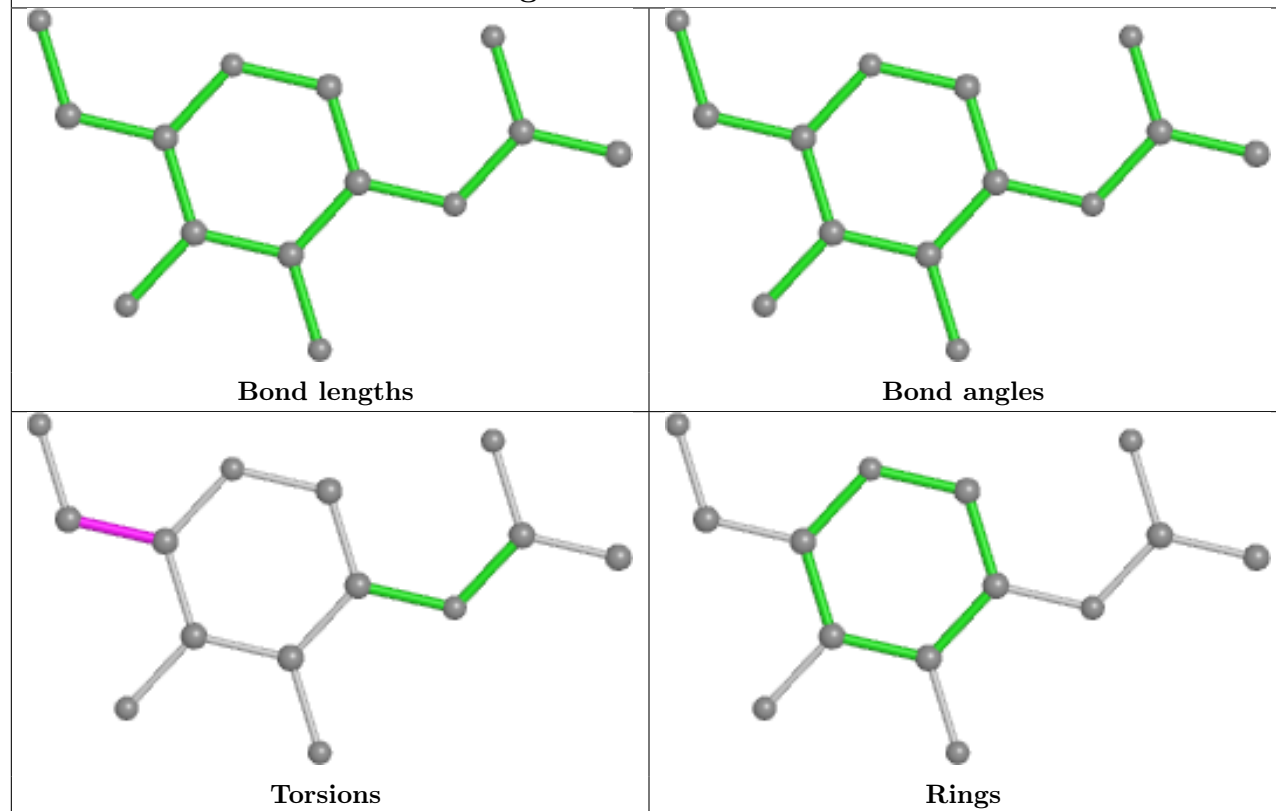


## Ligand NAG C 1408

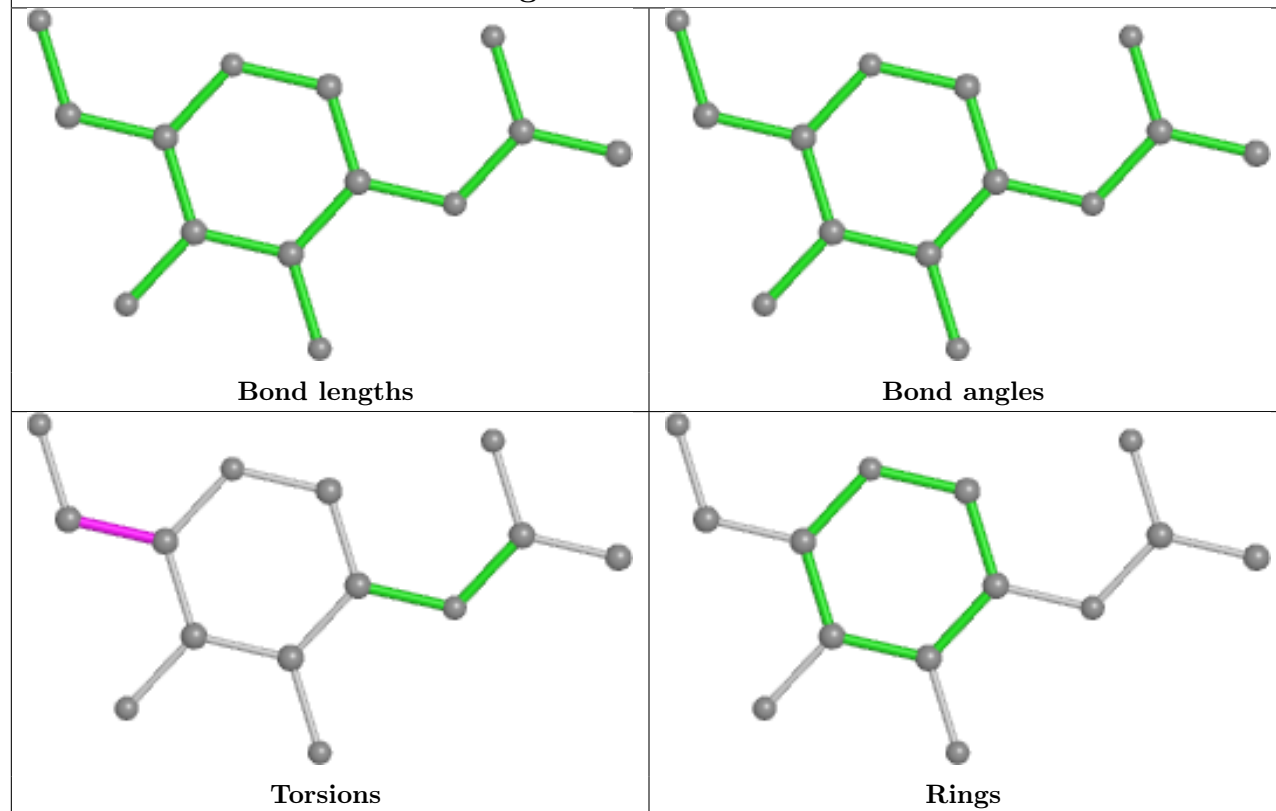


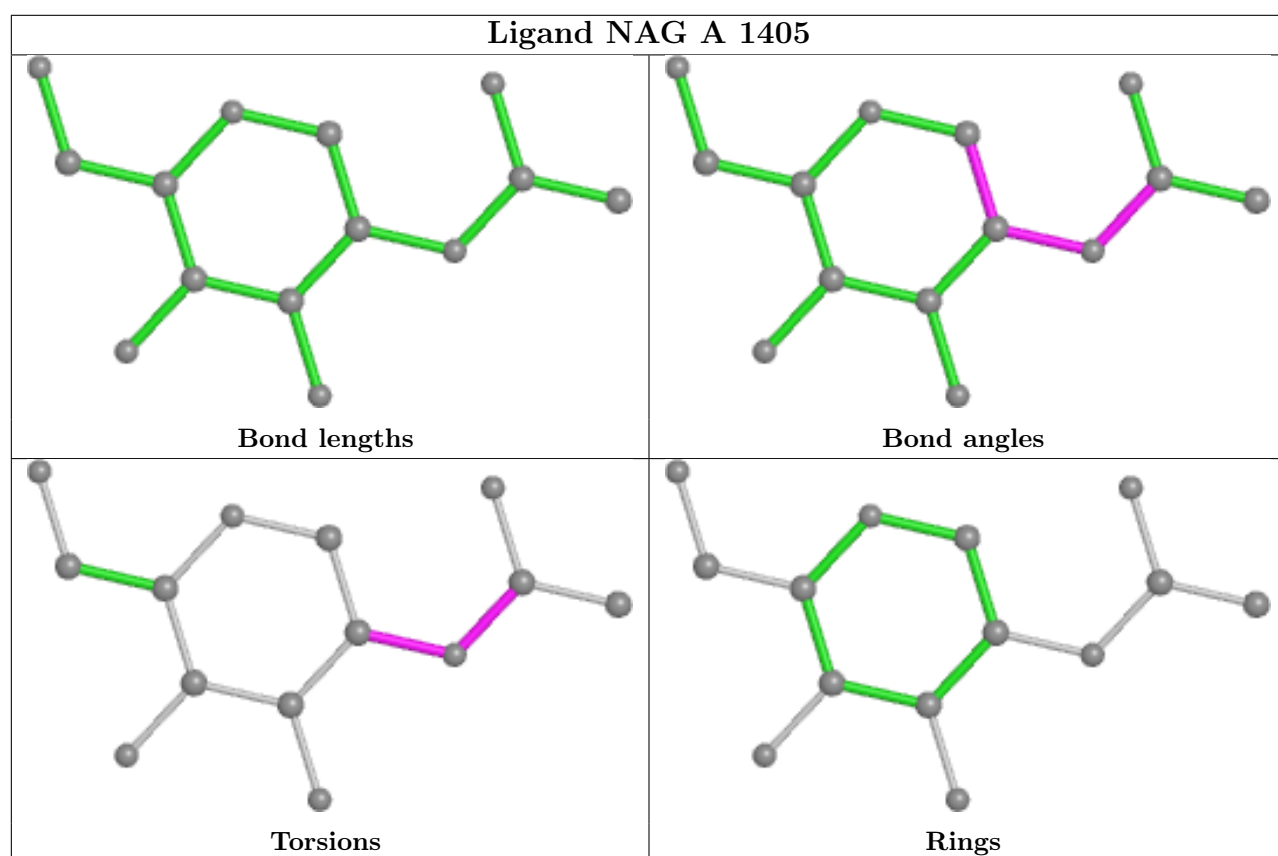
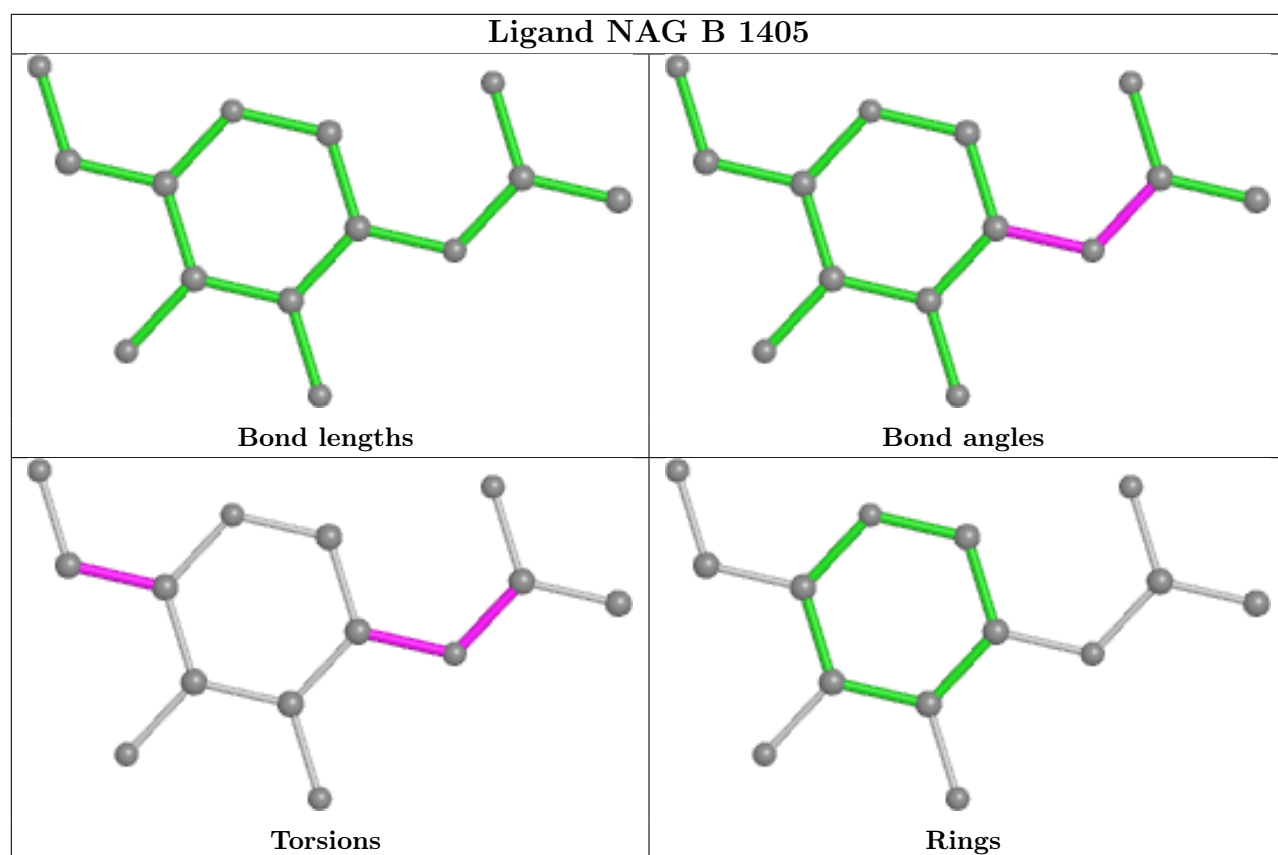


## Ligand NAG B 1406



## Ligand NAG C 1409





## 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.



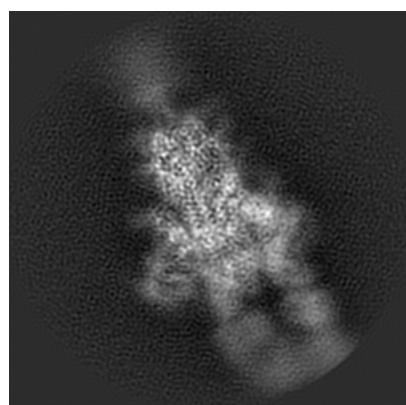
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30531. These allow visual inspection of the internal detail of the map and identification of artifacts.

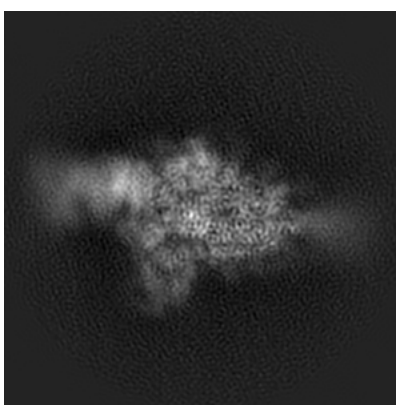
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

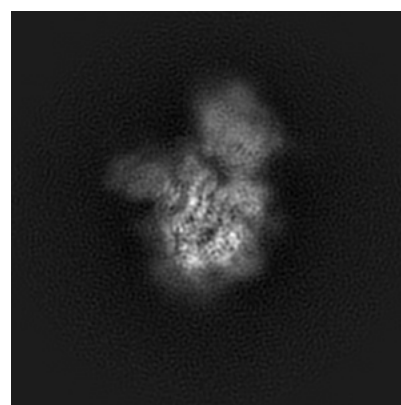
#### 6.1.1 Primary map



X



Y

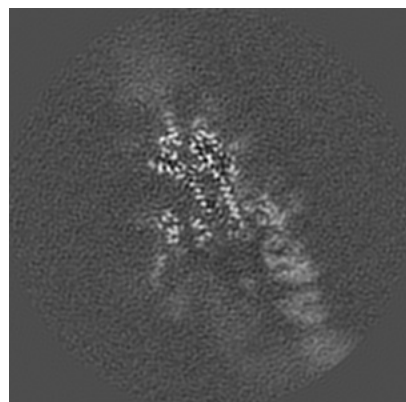


Z

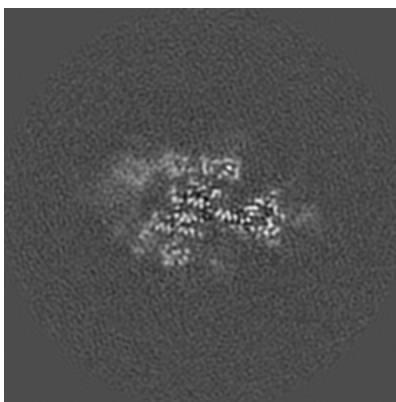
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

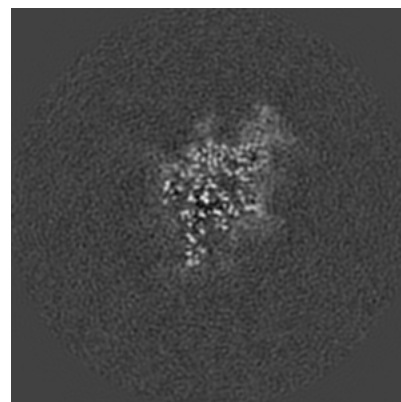
#### 6.2.1 Primary map



X Index: 144



Y Index: 144

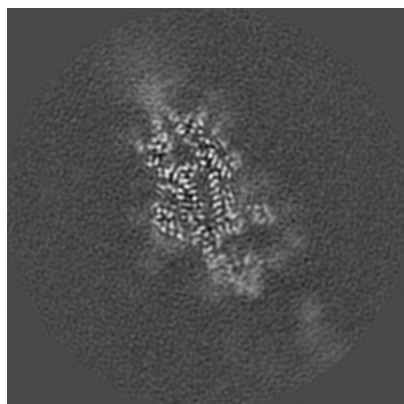


Z Index: 144

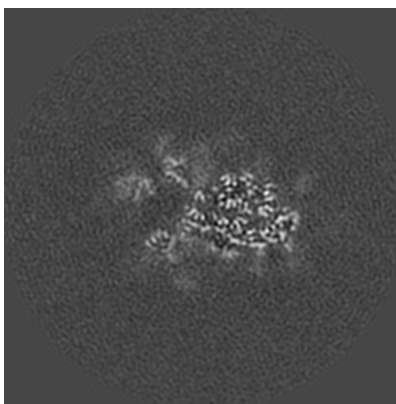
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

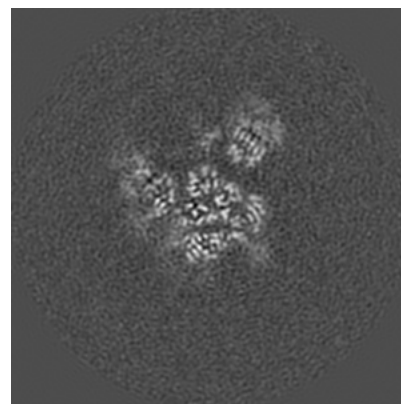
### 6.3.1 Primary map



X Index: 132



Y Index: 132

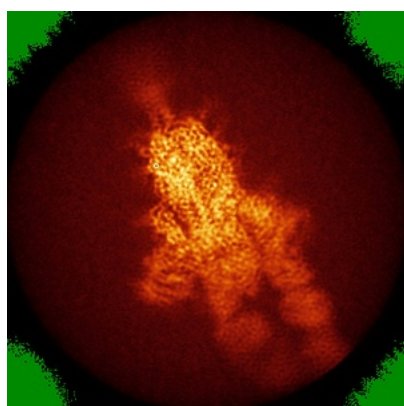


Z Index: 129

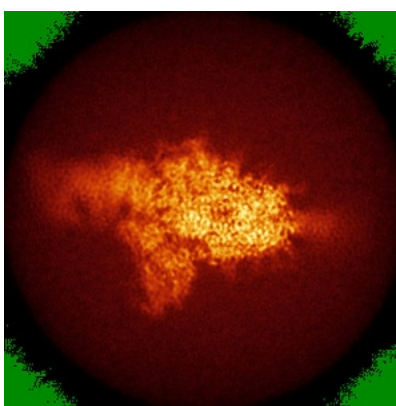
The images above show the largest variance slices of the map in three orthogonal directions.

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

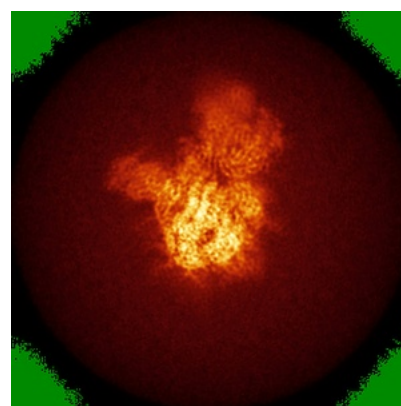
### 6.4.1 Primary map



X



Y

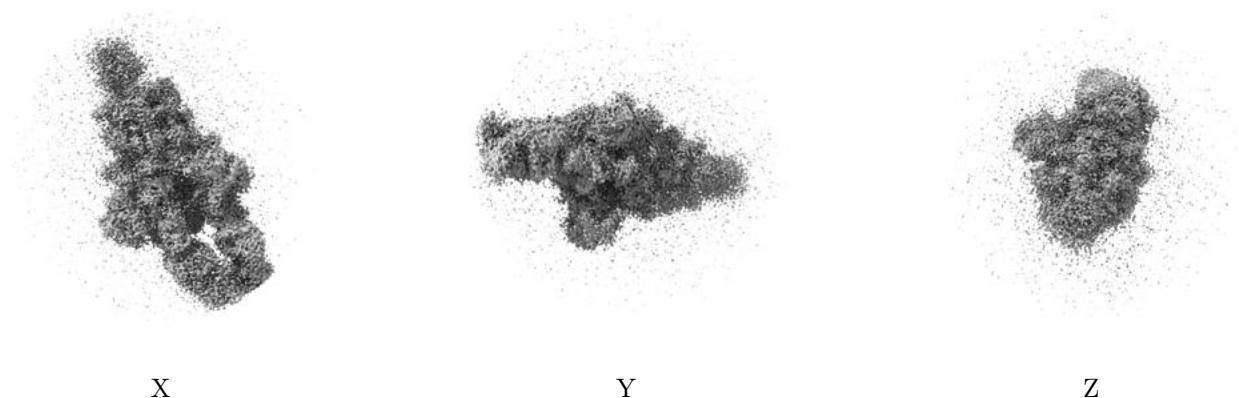


Z

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 0.0087. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

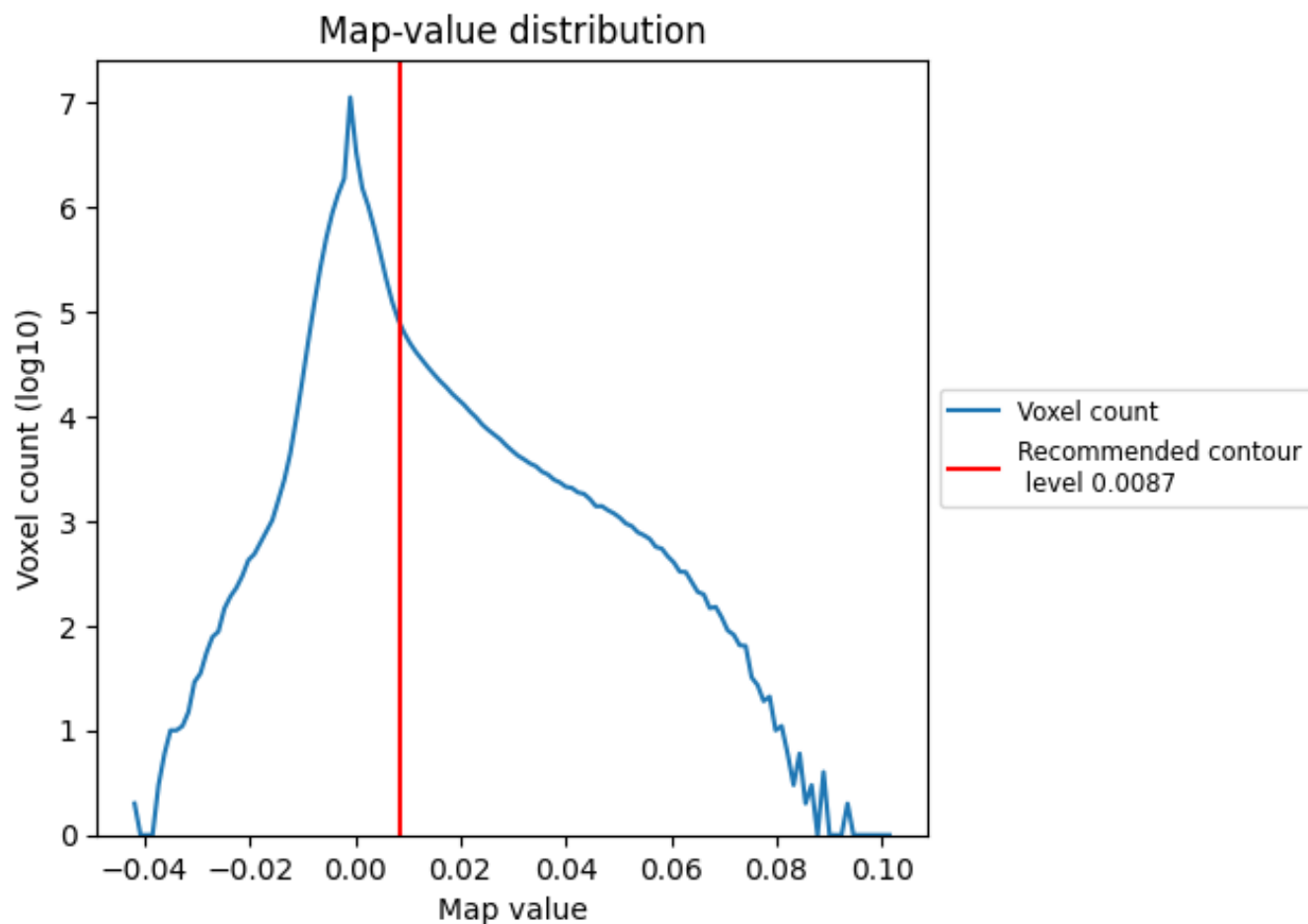
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

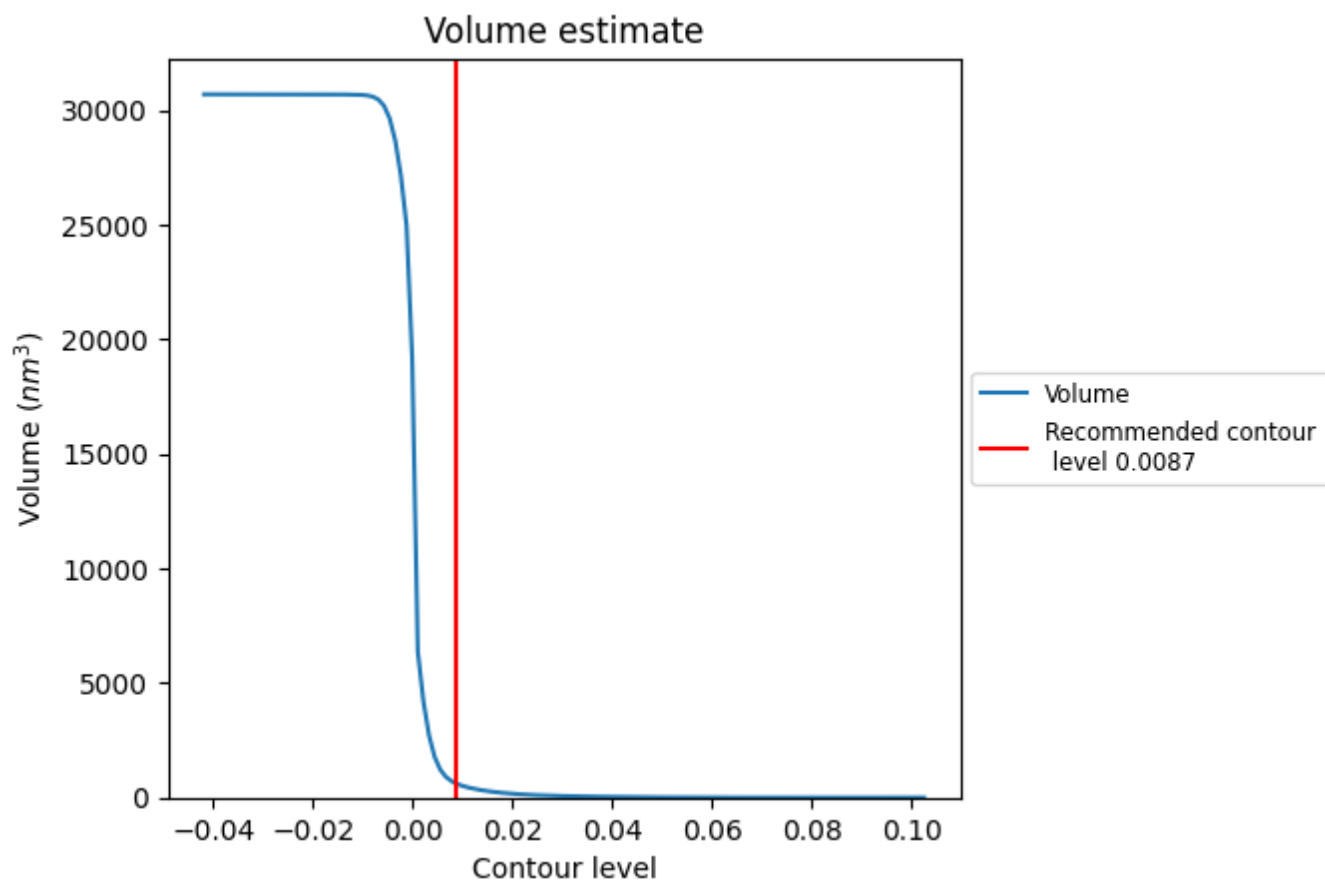
This section contains the results of statistical analysis of the map.

### 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.

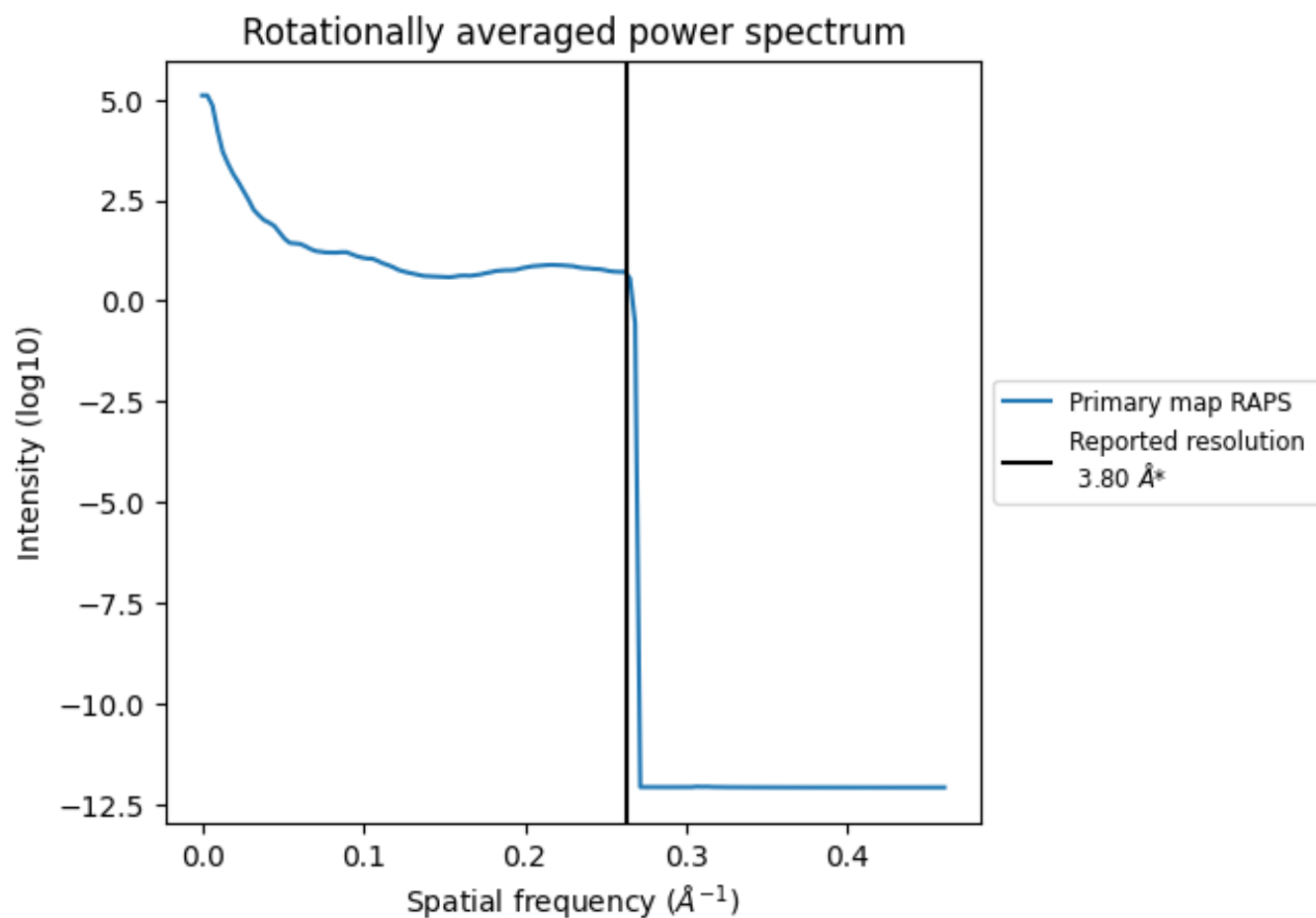
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 617 nm<sup>3</sup>; this corresponds to an approximate mass of 557 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 0.263 Å<sup>-1</sup>

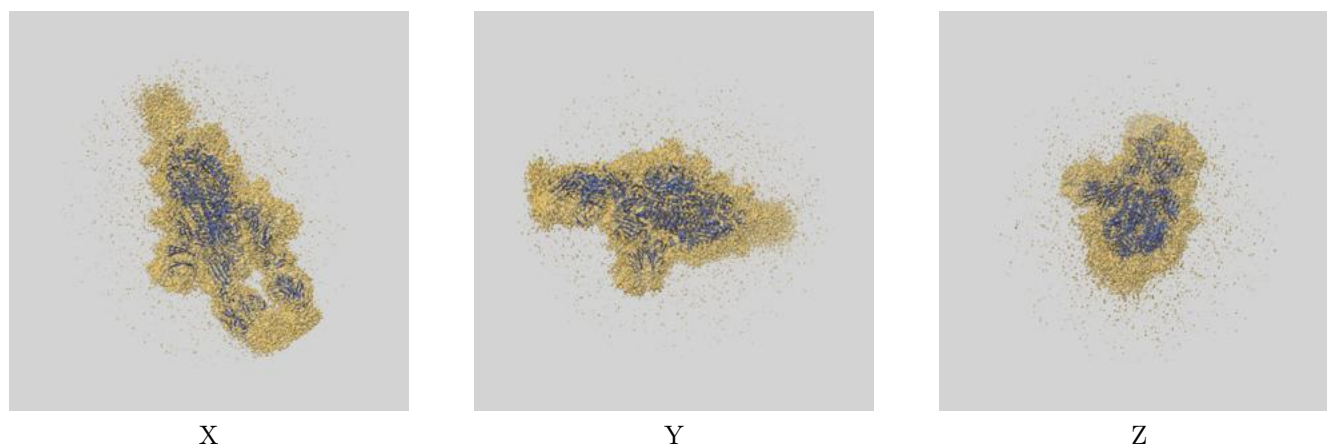
## 8 Fourier-Shell correlation ⓘ

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-30531 and PDB model 7D0D. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

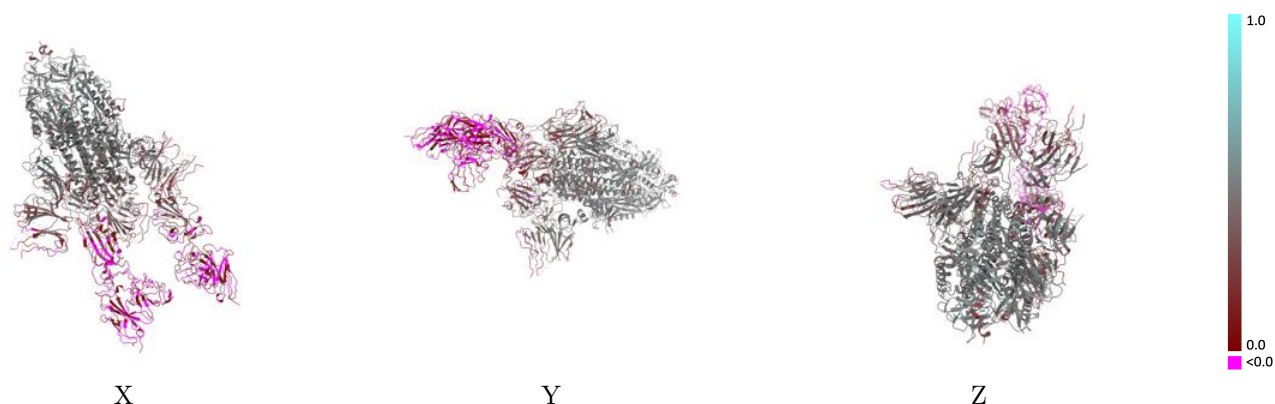
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0087 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.

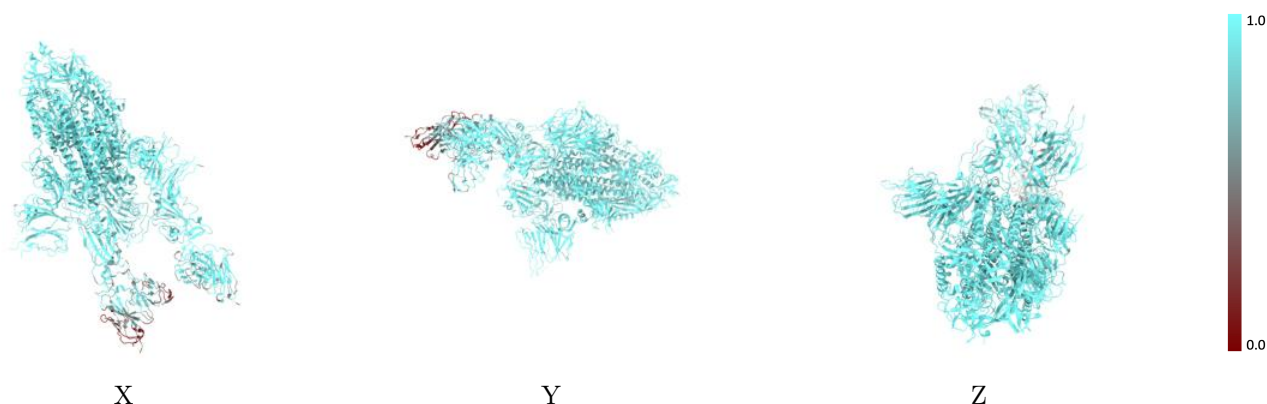


## 9.2 Q-score mapped to coordinate model [i](#)



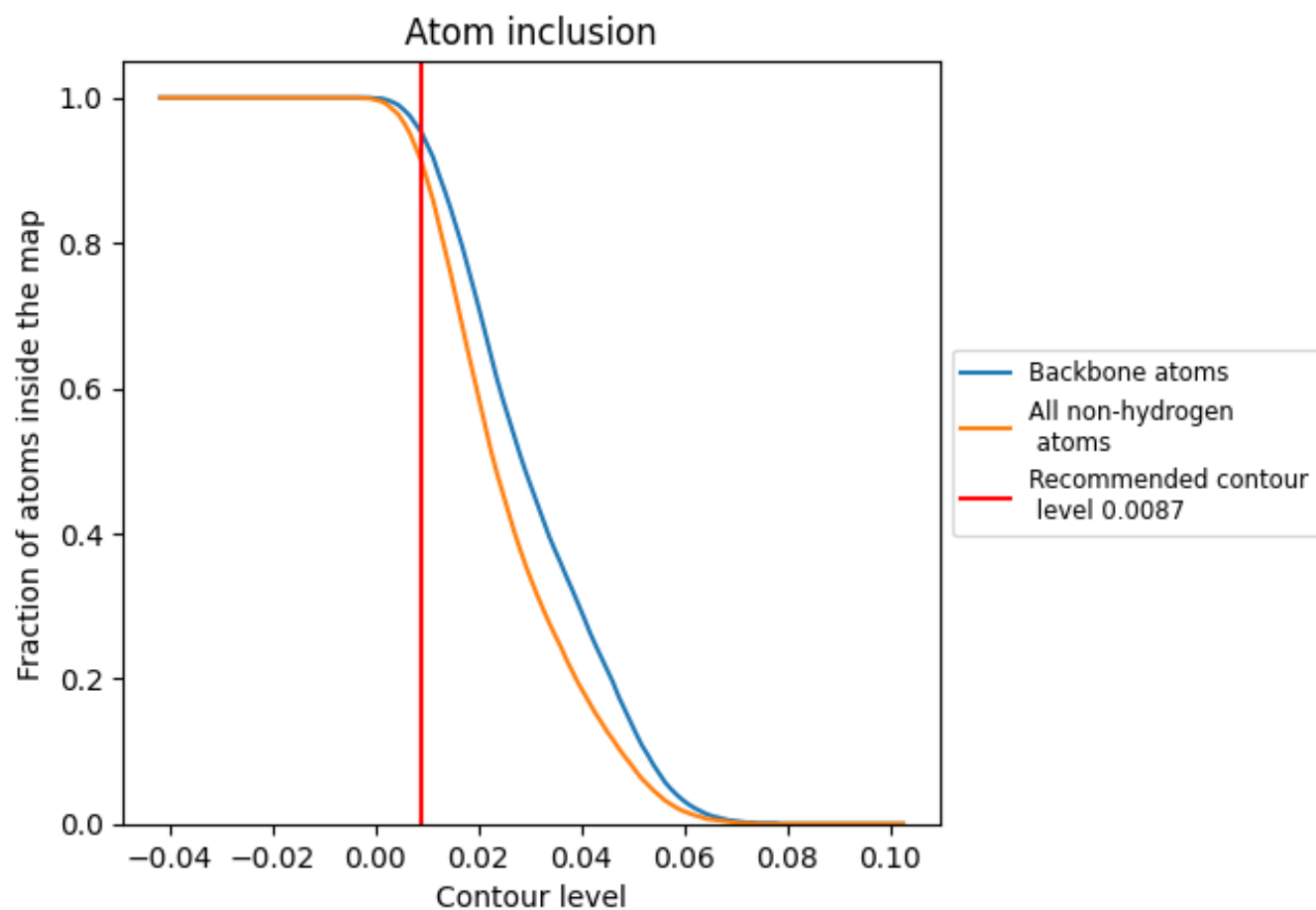
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0087).





























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.0087) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.3330
A	 0.9530	 0.3890
B	 0.9450	 0.3600
C	 0.9490	 0.3880
D	 0.9290	 0.3170
E	 0.8570	 0.1990
F	 0.6470	 0.0300
G	 0.4960	 0.0250
H	 0.8670	 0.0340
I	 0.8570	 0.2530
J	 0.9640	 0.4020
K	 0.9640	 0.3300
L	 0.8280	 0.0650
M	 0.8930	 0.2930
N	 1.0000	 0.4450
O	 1.0000	 0.3170
P	 0.5710	 0.1670
Q	 0.8210	 0.2180
R	 0.9290	 0.3960
S	 0.9290	 0.3260
T	 0.9640	 0.3430
U	 0.8930	 0.2410
V	 0.8570	 0.3370
W	 0.8210	 0.2260
X	 0.9290	 0.3700
Y	 0.9290	 0.3470
Z	 0.7500	 0.2840
a	 0.9290	 0.3930
b	 1.0000	 0.3010
c	 0.7500	 0.1650

