



## Full wwPDB EM Validation Report ⓘ

Apr 25, 2024 – 02:31 AM JST

PDB ID : 8Y1A  
EMDB ID : EMD-38829  
Title : 1up-1 conformation of HKU1-B S protein after incubation of the receptor  
Authors : Xia, L.Y.; Zhang, Y.Y.; Zhou, Q.  
Deposited on : 2024-01-24  
Resolution : 2.80 Å(reported)

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

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

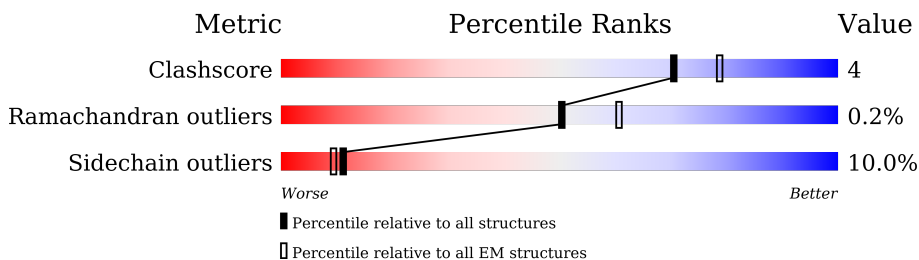
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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.



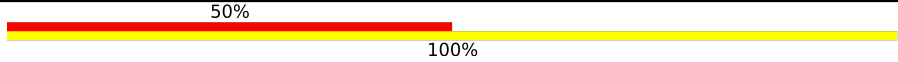
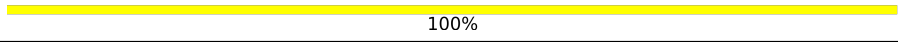
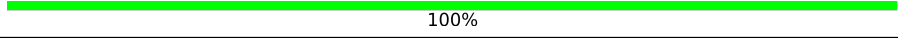
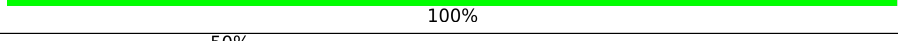


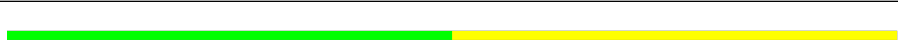

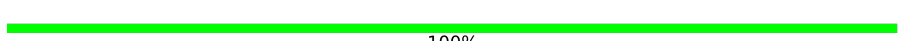

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1290	
1	B	1290	
1	C	1290	
2	D	6	
2	I	6	
2	N	6	
3	E	2	
3	F	2	

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Mol	Chain	Length	Quality of chain
3	G	2	 50% 100%
3	H	2	 100%
3	J	2	 100%
3	K	2	 100%
3	L	2	 50% 50%
3	M	2	 100%
3	O	2	 50% 50%
3	P	2	 50% 50%
3	Q	2	 50% 50%
3	R	2	 100%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29541 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.

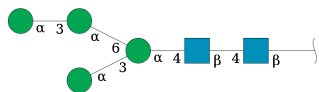
- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1208	9425	6003	1551	1814	57	0	0
1	B	1208	9425	6003	1551	1814	57	0	0
1	C	1208	9425	6003	1551	1814	57	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	752	GLY	ARG	conflict	UNP Q14EB0
A	753	SER	ARG	conflict	UNP Q14EB0
A	754	ALA	LYS	conflict	UNP Q14EB0
A	755	SER	ARG	conflict	UNP Q14EB0
A	1067	PRO	ASN	conflict	UNP Q14EB0
A	1068	PRO	LEU	conflict	UNP Q14EB0
B	752	GLY	ARG	conflict	UNP Q14EB0
B	753	SER	ARG	conflict	UNP Q14EB0
B	754	ALA	LYS	conflict	UNP Q14EB0
B	755	SER	ARG	conflict	UNP Q14EB0
B	1067	PRO	ASN	conflict	UNP Q14EB0
B	1068	PRO	LEU	conflict	UNP Q14EB0
C	752	GLY	ARG	conflict	UNP Q14EB0
C	753	SER	ARG	conflict	UNP Q14EB0
C	754	ALA	LYS	conflict	UNP Q14EB0
C	755	SER	ARG	conflict	UNP Q14EB0
C	1067	PRO	ASN	conflict	UNP Q14EB0
C	1068	PRO	LEU	conflict	UNP Q14EB0

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



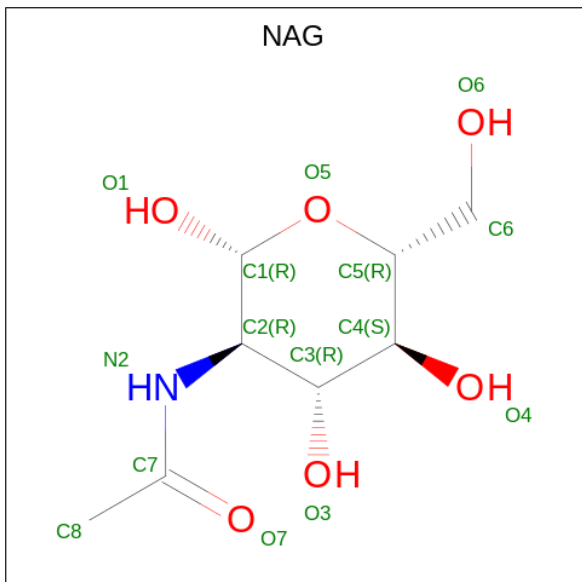
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	6	72	40	2	30	0	0
2	I	6	72	40	2	30	0	0
2	N	6	72	40	2	30	0	0

- Molecule 3 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
			Total	C	N	O		
3	E	2	28	16	2	10	0	0
3	F	2	28	16	2	10	0	0
3	G	2	28	16	2	10	0	0
3	H	2	28	16	2	10	0	0
3	J	2	28	16	2	10	0	0
3	K	2	28	16	2	10	0	0
3	L	2	28	16	2	10	0	0
3	M	2	28	16	2	10	0	0
3	O	2	28	16	2	10	0	0
3	P	2	28	16	2	10	0	0
3	Q	2	28	16	2	10	0	0
3	R	2	28	16	2	10	0	0

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



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

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

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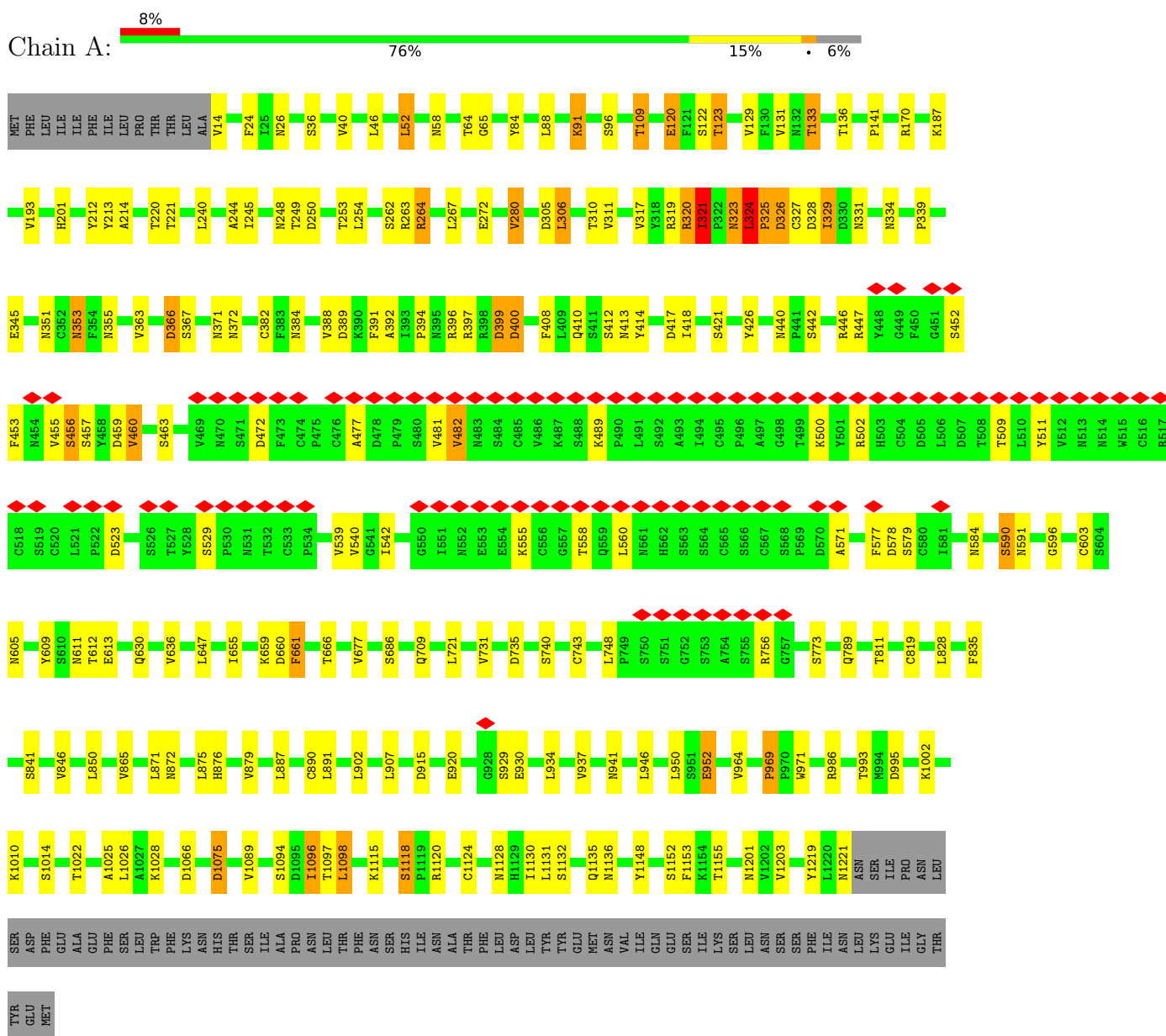




### 3 Residue-property plots [i](#)

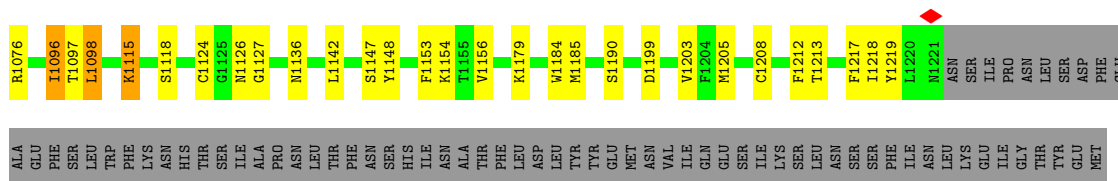
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Spike glycoprotein



#### • Molecule 1: Spike glycoprotein





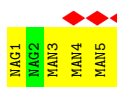
- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 33% 67%



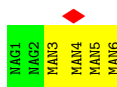
- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 17% 50% 83%



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

Chain N: 17% 33% 67%



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

Chain E: 100%



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

Chain F: 50% 50% 50%



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



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



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



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



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



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



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

Chain O:  50% 50%

NAG1  
NAG2

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

Chain P:  50% 50%

NAG1  
NAG2

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

Chain Q:  50% 50%

NAG1  
NAG2

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

Chain R:  100%

NAG1  
NAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150172	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.462	Depositor
Minimum map value	-2.895	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	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: MAN, 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	0.50	0/9653	0.59	1/13146 (0.0%)
1	B	0.47	0/9653	0.57	0/13146
1	C	0.51	0/9653	0.59	1/13146 (0.0%)
All	All	0.49	0/28959	0.58	2/39438 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	4
All	All	0	10

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	902	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	324	LEU	CA-CB-CG	5.31	127.50	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	819	CYS	Peptide
1	A	929	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	819	CYS	Peptide
1	B	92	PRO	Peptide
1	B	968	PHE	Peptide
1	B	969	PRO	Peptide
1	C	51	VAL	Peptide
1	C	819	CYS	Peptide
1	C	92	PRO	Peptide
1	C	969	PRO	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9425	0	9076	92	0
1	B	9425	0	9074	63	0
1	C	9425	0	9076	58	0
2	D	72	0	61	0	0
2	I	72	0	61	0	0
2	N	72	0	61	0	0
3	E	28	0	25	0	0
3	F	28	0	25	1	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
4	A	238	0	221	1	0
4	B	238	0	221	1	0
4	C	238	0	221	0	0
All	All	29541	0	28372	206	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 4.



All (206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASN:O	1:A:323:ASN:ND2	2.01	0.93
1:B:1132:SER:HG	1:B:1145:HIS:HD1	1.23	0.82
1:A:331:ASN:HD22	3:F:1:NAG:H81	1.56	0.71
1:A:306:LEU:HD23	1:A:677:VAL:O	1.93	0.69
1:A:320:ARG:C	1:A:321:ILE:HG13	2.11	0.69
1:B:201:HIS:HB2	1:B:212:TYR:HB2	1.78	0.66
1:A:326:ASP:OD1	1:A:326:ASP:N	2.27	0.65
1:B:79:LEU:HB2	1:B:239:PRO:HB3	1.79	0.64
1:C:201:HIS:HB2	1:C:212:TYR:HB2	1.79	0.64
1:A:306:LEU:HD23	1:A:306:LEU:N	2.13	0.64
1:A:324:LEU:HD13	1:A:351:ASN:C	2.19	0.63
1:A:1128:ASN:HB3	1:A:1148:TYR:HB3	1.81	0.63
1:A:389:ASP:O	1:A:590:SER:HA	2.00	0.62
1:A:872:ASN:H	1:A:876:HIS:HD2	1.47	0.62
1:A:306:LEU:HD23	1:A:306:LEU:H	1.63	0.62
1:A:326:ASP:HA	1:A:353:ASN:H	1.65	0.61
1:A:394:PRO:HB3	1:A:578:ASP:HB3	1.82	0.61
1:A:1025:ALA:HA	1:A:1028:LYS:HE3	1.83	0.61
1:B:262:SER:OG	1:B:264:ARG:NH1	2.34	0.60
1:A:201:HIS:HB2	1:A:212:TYR:HB2	1.84	0.60
1:C:214:ALA:HB2	1:C:220:THR:HA	1.84	0.59
1:B:415:LYS:HD3	1:B:542:ILE:HG13	1.85	0.59
1:B:952:GLU:HG3	1:B:1136:ASN:HD21	1.66	0.59
1:C:267:LEU:HB3	1:C:280:VAL:HG13	1.84	0.59
1:C:1126:ASN:ND2	1:C:1127:GLY:O	2.36	0.59
1:B:319:ARG:NH1	1:B:612:THR:O	2.36	0.58
1:C:872:ASN:H	1:C:876:HIS:HD2	1.49	0.58
1:A:267:LEU:HB3	1:A:280:VAL:HG13	1.86	0.57
1:A:400:ASP:O	1:A:410:GLN:NE2	2.36	0.57
1:C:952:GLU:HG3	1:C:1136:ASN:HD21	1.68	0.57
1:B:409:LEU:HA	1:B:413:ASN:HD22	1.69	0.57
1:B:214:ALA:HB2	1:B:220:THR:HA	1.86	0.57
1:A:320:ARG:O	1:A:321:ILE:HD12	2.05	0.57
1:C:132:ASN:OD1	1:C:132:ASN:N	2.34	0.57
1:C:192:ASN:HB3	1:C:195:ALA:HB2	1.86	0.56
1:A:459:ASP:HA	1:A:579:SER:HA	1.88	0.56
1:A:611:ASN:HB2	1:A:613:GLU:HG2	1.88	0.55
1:B:482:VAL:O	1:B:489:LYS:NZ	2.40	0.55
1:B:1108:GLU:OE1	1:B:1120:ARG:NH2	2.40	0.55
1:A:323:ASN:O	1:A:324:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:SER:OG	1:B:457:SER:N	2.39	0.55
1:A:396:ARG:NH2	1:A:577:PHE:O	2.40	0.55
1:B:791:PRO:HB3	1:B:1150:PRO:HB3	1.89	0.55
1:A:709:GLN:HG3	1:A:721:LEU:HD13	1.89	0.54
1:B:73:ASN:HD22	1:B:74:PHE:H	1.56	0.54
1:C:22:ASN:N	1:C:22:ASN:OD1	2.41	0.54
1:C:846:VAL:HG13	1:C:1096:ILE:HG13	1.88	0.54
1:A:319:ARG:NH1	1:A:611:ASN:O	2.41	0.53
1:C:472:ASP:OD1	1:C:472:ASP:N	2.40	0.53
1:B:879:VAL:HG21	1:B:967:MET:HB3	1.89	0.53
1:C:356:LEU:HD12	1:C:359:LEU:HD23	1.91	0.53
1:A:477:ALA:HA	1:A:502:ARG:HB3	1.91	0.53
1:A:482:VAL:O	1:A:489:LYS:NZ	2.42	0.53
1:A:345:GLU:O	1:A:389:ASP:HA	2.09	0.52
1:A:262:SER:OG	1:A:264:ARG:NH1	2.43	0.52
1:C:680:ALA:HB1	1:C:736:LEU:HD13	1.92	0.52
1:C:396:ARG:NH2	1:C:577:PHE:O	2.43	0.52
1:A:413:ASN:HD21	1:A:463:SER:H	1.58	0.52
1:B:1182:ASP:OD1	1:B:1182:ASP:N	2.43	0.51
1:A:306:LEU:N	1:A:306:LEU:CD2	2.73	0.51
1:C:863:GLN:O	1:C:1115:LYS:NZ	2.43	0.51
1:B:353:ASN:HB3	1:B:605:ASN:HD22	1.74	0.51
1:B:692:TYR:HB3	1:B:695:LEU:HD12	1.91	0.51
1:C:570:ASP:OD1	1:C:570:ASP:N	2.42	0.51
1:A:131:VAL:HG11	1:C:447:ARG:HD2	1.92	0.51
1:A:408:PHE:O	1:A:412:SER:HB2	2.10	0.51
1:B:417:ASP:OD2	1:C:206:ARG:NH2	2.42	0.51
1:C:828:LEU:HD11	1:C:1071:GLN:HG2	1.93	0.51
1:B:151:CYS:HA	1:B:183:CYS:HA	1.93	0.50
1:B:109:THR:HG21	1:B:254:LEU:HD22	1.94	0.50
1:A:327:CYS:N	1:A:353:ASN:O	2.41	0.50
1:A:339:PRO:HG2	1:A:391:PHE:HA	1.92	0.50
1:A:1098:LEU:HD13	1:B:1097:THR:HG23	1.93	0.50
1:B:552:ASN:HB2	1:B:573:LEU:HD21	1.94	0.50
1:C:907:LEU:HD11	1:C:1142:LEU:HD22	1.94	0.50
1:C:552:ASN:HB2	1:C:573:LEU:HD11	1.93	0.50
1:C:1205:MET:HE1	1:C:1212:PHE:HE2	1.76	0.49
1:C:332:TRP:O	1:C:390:LYS:NZ	2.38	0.49
1:C:482:VAL:O	1:C:489:LYS:NZ	2.45	0.49
1:A:400:ASP:N	1:A:400:ASP:OD1	2.46	0.49
1:B:442:SER:HB3	1:B:445:ASN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:LEU:HD13	1:B:1096:ILE:HD11	1.95	0.49
1:B:161:THR:HA	1:B:172:GLU:HG3	1.95	0.49
1:B:21:THR:OG1	1:B:22:ASN:N	2.46	0.49
1:B:1196:PRO:O	1:B:1201:ASN:ND2	2.45	0.49
1:A:399:ASP:N	1:A:399:ASP:OD1	2.46	0.48
1:A:456:SER:OG	1:A:457:SER:N	2.45	0.48
1:A:846:VAL:HG13	1:A:1096:ILE:HG13	1.94	0.48
1:C:740:SER:O	1:C:740:SER:OG	2.31	0.48
1:B:103:PHE:HB2	1:B:261:LEU:HD21	1.96	0.48
1:B:570:ASP:OD1	1:B:570:ASP:N	2.42	0.48
1:A:133:THR:O	1:C:446:ARG:NH2	2.47	0.48
1:B:900:ARG:NH1	1:B:905:ASP:OD1	2.47	0.48
1:C:399:ASP:N	1:C:399:ASP:OD1	2.44	0.48
1:A:65:GLY:O	1:A:263:ARG:HA	2.14	0.47
1:A:442:SER:O	1:A:446:ARG:NE	2.46	0.47
1:A:123:THR:HG22	1:A:141:PRO:HD2	1.97	0.47
1:A:120:GLU:HG2	1:A:240:LEU:HD21	1.97	0.47
1:A:440:ASN:HD21	1:A:442:SER:HB3	1.80	0.47
1:B:508:THR:HG23	1:B:513:ASN:HA	1.96	0.47
1:C:345:GLU:O	1:C:389:ASP:HA	2.15	0.47
1:A:636:VAL:O	1:A:666:THR:OG1	2.32	0.47
1:B:430:PRO:HG3	1:B:585:ARG:HH21	1.80	0.47
1:B:19:ASN:HB3	1:B:157:GLU:CD	2.35	0.47
1:A:789:GLN:NE2	1:A:1155:THR:OG1	2.48	0.46
1:A:367:SER:HB3	1:A:426:TYR:HD2	1.79	0.46
1:A:382:CYS:HA	1:A:603:CYS:HA	1.97	0.46
1:A:452:SER:OG	1:A:453:PHE:N	2.49	0.46
1:C:512:VAL:HG12	1:C:514:ASN:H	1.80	0.46
1:A:366:ASP:N	1:A:366:ASP:OD1	2.49	0.46
1:A:388:VAL:HA	1:A:591:ASN:O	2.15	0.46
1:A:937:VAL:O	1:A:941:ASN:ND2	2.36	0.46
1:B:1098:LEU:HD13	1:C:1097:THR:HG23	1.96	0.46
1:B:132:ASN:OD1	1:B:132:ASN:N	2.49	0.46
1:A:372:ASN:HB2	1:A:421:SER:HA	1.97	0.46
1:C:340:SER:OG	1:C:343:ASN:OD1	2.34	0.46
1:A:214:ALA:HB2	1:A:220:THR:HA	1.98	0.46
1:A:355:ASN:HA	1:A:605:ASN:HB3	1.97	0.45
1:A:417:ASP:HB2	1:A:542:ILE:HG21	1.98	0.45
1:B:187:LYS:O	1:B:188:ASN:OD1	2.34	0.45
1:C:1148:TYR:OH	1:C:1190:SER:O	2.31	0.45
1:A:324:LEU:HB3	1:A:325:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PHE:HB2	1:A:170:ARG:HH12	1.80	0.45
1:B:163:CYS:HB3	1:B:240:LEU:HD11	1.99	0.45
1:C:743:CYS:HB3	1:C:765:VAL:HG23	1.98	0.45
1:A:952:GLU:HG3	1:A:1136:ASN:HD21	1.81	0.45
1:B:478:ASP:HB3	1:B:481:VAL:HG23	1.98	0.45
1:B:537:LYS:HB2	1:B:537:LYS:HE3	1.73	0.45
1:A:317:VAL:HA	1:A:611:ASN:HD21	1.82	0.45
1:A:372:ASN:ND2	1:A:418:ILE:O	2.50	0.45
1:A:555:LYS:HD2	1:A:571:ALA:HB2	1.99	0.45
1:A:969:PRO:HA	1:A:971:TRP:CE2	2.52	0.45
1:A:392:ALA:HB3	1:A:460:VAL:HG11	1.99	0.45
1:B:795:THR:OG1	1:B:796:ILE:N	2.49	0.45
1:C:735:ASP:OD1	1:C:735:ASP:N	2.43	0.45
1:B:523:ASP:OD1	1:B:526:SER:OG	2.35	0.44
1:B:187:LYS:HD2	1:B:188:ASN:H	1.82	0.44
1:B:1218:ILE:HG23	1:B:1220:LEU:HB2	1.99	0.44
1:B:902:LEU:HA	1:B:905:ASP:HB2	2.00	0.44
1:B:969:PRO:HA	1:B:971:TRP:CE2	2.53	0.44
1:A:328:ASP:OD1	1:A:328:ASP:N	2.45	0.44
1:B:91:LYS:HB3	1:B:93:PRO:HD2	1.98	0.44
1:B:213:TYR:HB3	1:B:223:LEU:HD22	1.99	0.44
1:C:496:PRO:O	1:C:499:THR:OG1	2.33	0.44
1:A:26:ASN:HB2	1:A:84:TYR:HB3	2.00	0.44
1:C:1184:TRP:HB2	1:C:1218:ILE:HD11	1.99	0.44
1:C:215:ASP:OD1	1:C:215:ASP:N	2.51	0.44
1:A:647:LEU:HD22	1:A:655:ILE:HD11	2.00	0.44
1:A:389:ASP:OD2	1:A:414:TYR:OH	2.29	0.43
1:A:459:ASP:HB3	1:A:577:PHE:HD2	1.84	0.43
1:A:1118:SER:HB3	1:A:1120:ARG:H	1.83	0.43
1:C:789:GLN:HG3	1:C:1153:PHE:HB3	2.01	0.43
1:A:88:LEU:HA	1:A:91:LYS:HE2	2.00	0.43
1:C:478:ASP:HB3	1:C:481:VAL:HG23	2.00	0.43
1:B:1173:LYS:HG3	1:B:1203:VAL:HG12	2.00	0.43
1:C:758:ILE:H	1:C:758:ILE:HG13	1.47	0.43
1:B:487:LYS:HB2	1:B:515:TRP:HB2	2.00	0.43
1:C:789:GLN:HA	1:C:1154:LYS:O	2.17	0.43
1:C:431:LEU:O	1:C:458:TYR:OH	2.30	0.43
1:A:320:ARG:C	1:A:321:ILE:CG1	2.84	0.43
1:A:789:GLN:HG3	1:A:1153:PHE:HB3	2.00	0.43
1:B:995:ASP:N	1:B:995:ASP:OD1	2.52	0.42
1:A:472:ASP:HB2	1:A:500:LYS:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:561:ASN:HD22	1:C:562:HIS:H	1.67	0.42
1:C:508:THR:HG23	1:C:513:ASN:HA	2.01	0.42
1:C:124:ILE:HG13	1:C:237:VAL:HG22	2.00	0.42
1:B:872:ASN:HD21	1:B:894:GLN:HE21	1.68	0.42
1:A:920:GLU:HG3	4:A:2016:NAG:H82	2.02	0.42
1:B:1091:GLN:HE21	1:B:1091:GLN:HB3	1.51	0.42
1:C:149:THR:HG22	1:C:186:LYS:HG3	2.00	0.42
1:A:319:ARG:NH2	1:A:660:ASP:OD2	2.53	0.42
1:A:887:LEU:O	1:A:1135:GLN:NE2	2.50	0.42
1:A:1075:ASP:OD2	1:C:1076:ARG:NH2	2.41	0.42
1:B:194:SER:OG	4:B:2006:NAG:O7	2.35	0.42
1:B:162:VAL:HB	1:B:172:GLU:HB2	2.02	0.42
1:C:362:LEU:HD23	1:C:362:LEU:HA	1.94	0.42
1:C:1064:ARG:HE	1:C:1064:ARG:HB3	1.56	0.42
1:A:244:ALA:HA	1:A:249:THR:HG21	2.02	0.41
1:B:1132:SER:HA	1:B:1144:ILE:O	2.20	0.41
1:A:109:THR:HG21	1:A:254:LEU:HD23	2.02	0.41
1:B:1197:ILE:HA	1:B:1201:ASN:HD22	1.85	0.41
1:C:104:SER:HA	1:C:257:TRP:O	2.19	0.41
1:A:396:ARG:HG3	1:A:397:ARG:HG2	2.02	0.41
1:B:123:THR:HG22	1:B:141:PRO:HD2	2.03	0.41
1:C:1012:LEU:HD23	1:C:1012:LEU:HA	1.88	0.41
1:A:52:LEU:H	1:A:52:LEU:HG	1.52	0.41
1:A:384:ASN:HB2	1:A:596:GLY:HA3	2.02	0.41
1:C:843:LEU:HD23	1:C:843:LEU:HA	1.95	0.41
1:C:358:THR:HA	1:C:361:ARG:HG2	2.02	0.41
1:C:969:PRO:HA	1:C:971:TRP:CE2	2.56	0.41
1:A:661:PHE:HD1	1:A:661:PHE:HA	1.76	0.41
1:A:1130:ILE:HG22	1:A:1131:LEU:HD23	2.03	0.41
1:B:559:GLN:HB3	1:B:560:LEU:HD23	2.03	0.41
1:A:523:ASP:OD1	1:A:523:ASP:N	2.54	0.41
1:A:329:ILE:H	1:A:329:ILE:HG13	1.56	0.40
1:A:1097:THR:HG23	1:C:1098:LEU:HD13	2.02	0.40
1:B:223:LEU:HA	1:B:223:LEU:HD12	1.85	0.40
1:B:1184:TRP:HB2	1:B:1218:ILE:HD11	2.03	0.40
1:B:1218:ILE:HA	1:B:1220:LEU:HD23	2.04	0.40
1:C:523:ASP:OD1	1:C:523:ASP:N	2.53	0.40
1:A:355:ASN:OD1	1:A:605:ASN:ND2	2.42	0.40
1:C:366:ASP:OD1	1:C:366:ASP:N	2.53	0.40
1:A:740:SER:O	1:A:740:SER:OG	2.34	0.40
1:A:995:ASP:OD1	1:A:995:ASP:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:LYS:NZ	1:B:851:ASP:OD1	2.36	0.40
1:C:110:LYS:HB3	1:C:117:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1206/1290 (94%)	1118 (93%)	84 (7%)	4 (0%)	41 72
1	B	1206/1290 (94%)	1118 (93%)	87 (7%)	1 (0%)	51 81
1	C	1206/1290 (94%)	1136 (94%)	68 (6%)	2 (0%)	47 78
All	All	3618/3870 (94%)	3372 (93%)	239 (7%)	7 (0%)	50 78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	ILE
1	A	36	SER
1	A	324	LEU
1	B	172	GLU
1	C	250	ASP
1	C	36	SER
1	A	325	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1082/1159 (93%)	970 (90%)	112 (10%)	7	21
1	B	1082/1159 (93%)	969 (90%)	113 (10%)	7	21
1	C	1082/1159 (93%)	982 (91%)	100 (9%)	9	27
All	All	3246/3477 (93%)	2921 (90%)	325 (10%)	11	22

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	40	VAL
1	A	46	LEU
1	A	52	LEU
1	A	58	ASN
1	A	64	THR
1	A	91	LYS
1	A	96	SER
1	A	109	THR
1	A	120	GLU
1	A	122	SER
1	A	123	THR
1	A	129	VAL
1	A	133	THR
1	A	136	THR
1	A	187	LYS
1	A	193	VAL
1	A	213	TYR
1	A	221	THR
1	A	245	ILE
1	A	248	ASN
1	A	250	ASP
1	A	253	THR
1	A	264	ARG
1	A	272	GLU
1	A	280	VAL
1	A	305	ASP
1	A	306	LEU
1	A	310	THR
1	A	311	VAL
1	A	320	ARG
1	A	321	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	323	ASN
1	A	326	ASP
1	A	329	ILE
1	A	334	ASN
1	A	353	ASN
1	A	363	VAL
1	A	366	ASP
1	A	371	ASN
1	A	399	ASP
1	A	400	ASP
1	A	447	ARG
1	A	455	VAL
1	A	456	SER
1	A	460	VAL
1	A	481	VAL
1	A	482	VAL
1	A	509	THR
1	A	511	TYR
1	A	529	SER
1	A	539	VAL
1	A	540	VAL
1	A	558	THR
1	A	560	LEU
1	A	584	ASN
1	A	590	SER
1	A	609	TYR
1	A	612	THR
1	A	630	GLN
1	A	659	LYS
1	A	661	PHE
1	A	686	SER
1	A	731	VAL
1	A	735	ASP
1	A	743	CYS
1	A	748	LEU
1	A	756	ARG
1	A	773	SER
1	A	811	THR
1	A	828	LEU
1	A	835	PHE
1	A	841	SER
1	A	850	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	865	VAL
1	A	871	LEU
1	A	875	LEU
1	A	879	VAL
1	A	890	CYS
1	A	891	LEU
1	A	902	LEU
1	A	907	LEU
1	A	915	ASP
1	A	930	GLU
1	A	934	LEU
1	A	946	LEU
1	A	950	LEU
1	A	952	GLU
1	A	964	VAL
1	A	969	PRO
1	A	986	ARG
1	A	993	THR
1	A	1002	LYS
1	A	1010	LYS
1	A	1014	SER
1	A	1022	THR
1	A	1026	LEU
1	A	1066	ASP
1	A	1075	ASP
1	A	1089	VAL
1	A	1094	SER
1	A	1096	ILE
1	A	1098	LEU
1	A	1115	LYS
1	A	1118	SER
1	A	1124	CYS
1	A	1132	SER
1	A	1152	SER
1	A	1201	ASN
1	A	1203	VAL
1	A	1219	TYR
1	A	1221	ASN
1	B	14	VAL
1	B	17	ASP
1	B	28	TYR
1	B	29	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	30	LYS
1	B	32	ILE
1	B	34	ARG
1	B	35	ILE
1	B	38	ASP
1	B	51	VAL
1	B	52	LEU
1	B	57	LEU
1	B	58	ASN
1	B	73	ASN
1	B	85	LEU
1	B	87	THR
1	B	120	GLU
1	B	123	THR
1	B	124	ILE
1	B	131	VAL
1	B	132	ASN
1	B	136	THR
1	B	149	THR
1	B	187	LYS
1	B	198	LEU
1	B	204	GLN
1	B	205	GLU
1	B	208	VAL
1	B	213	TYR
1	B	215	ASP
1	B	221	THR
1	B	250	ASP
1	B	253	THR
1	B	254	LEU
1	B	259	THR
1	B	263	ARG
1	B	264	ARG
1	B	310	THR
1	B	324	LEU
1	B	363	VAL
1	B	369	SER
1	B	373	LEU
1	B	374	ASP
1	B	418	ILE
1	B	434	VAL
1	B	447	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	455	VAL
1	B	460	VAL
1	B	468	SER
1	B	480	SER
1	B	481	VAL
1	B	511	TYR
1	B	517	ARG
1	B	527	THR
1	B	537	LYS
1	B	560	LEU
1	B	570	ASP
1	B	573	LEU
1	B	584	ASN
1	B	601	THR
1	B	644	TRP
1	B	654	ASN
1	B	655	ILE
1	B	659	LYS
1	B	706	PHE
1	B	731	VAL
1	B	735	ASP
1	B	743	CYS
1	B	758	ILE
1	B	763	ARG
1	B	779	VAL
1	B	788	ILE
1	B	811	THR
1	B	815	SER
1	B	831	GLU
1	B	835	PHE
1	B	841	SER
1	B	849	LEU
1	B	850	LEU
1	B	865	VAL
1	B	871	LEU
1	B	879	VAL
1	B	885	LYS
1	B	902	LEU
1	B	905	ASP
1	B	929	SER
1	B	930	GLU
1	B	950	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	952	GLU
1	B	953	THR
1	B	964	VAL
1	B	986	ARG
1	B	995	ASP
1	B	1012	LEU
1	B	1026	LEU
1	B	1033	VAL
1	B	1055	SER
1	B	1058	LEU
1	B	1063	SER
1	B	1066	ASP
1	B	1086	ASN
1	B	1091	GLN
1	B	1094	SER
1	B	1096	ILE
1	B	1098	LEU
1	B	1117	GLN
1	B	1118	SER
1	B	1124	CYS
1	B	1147	SER
1	B	1156	VAL
1	B	1182	ASP
1	B	1203	VAL
1	B	1219	TYR
1	C	14	VAL
1	C	23	SER
1	C	31	THR
1	C	32	ILE
1	C	34	ARG
1	C	52	LEU
1	C	57	LEU
1	C	96	SER
1	C	104	SER
1	C	111	LEU
1	C	120	GLU
1	C	122	SER
1	C	123	THR
1	C	132	ASN
1	C	175	HIS
1	C	187	LYS
1	C	193	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	213	TYR
1	C	221	THR
1	C	245	ILE
1	C	255	GLU
1	C	280	VAL
1	C	289	GLU
1	C	305	ASP
1	C	319	ARG
1	C	369	SER
1	C	373	LEU
1	C	375	LYS
1	C	399	ASP
1	C	418	ILE
1	C	428	SER
1	C	460	VAL
1	C	481	VAL
1	C	482	VAL
1	C	528	TYR
1	C	529	SER
1	C	560	LEU
1	C	561	ASN
1	C	570	ASP
1	C	584	ASN
1	C	608	LEU
1	C	612	THR
1	C	618	VAL
1	C	635	GLU
1	C	655	ILE
1	C	659	LYS
1	C	662	LEU
1	C	668	THR
1	C	670	LEU
1	C	676	ARG
1	C	698	SER
1	C	726	LEU
1	C	735	ASP
1	C	748	LEU
1	C	750	SER
1	C	758	ILE
1	C	778	SER
1	C	779	VAL
1	C	780	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	820	SER
1	C	845	GLU
1	C	850	LEU
1	C	854	GLN
1	C	865	VAL
1	C	871	LEU
1	C	879	VAL
1	C	885	LYS
1	C	894	GLN
1	C	895	CYS
1	C	902	LEU
1	C	903	LEU
1	C	929	SER
1	C	930	GLU
1	C	952	GLU
1	C	953	THR
1	C	964	VAL
1	C	972	SER
1	C	977	VAL
1	C	981	LEU
1	C	1001	GLN
1	C	1022	THR
1	C	1026	LEU
1	C	1030	GLN
1	C	1066	ASP
1	C	1075	ASP
1	C	1096	ILE
1	C	1098	LEU
1	C	1115	LYS
1	C	1118	SER
1	C	1124	CYS
1	C	1147	SER
1	C	1156	VAL
1	C	1179	LYS
1	C	1185	MET
1	C	1199	ASP
1	C	1203	VAL
1	C	1208	CYS
1	C	1213	THR
1	C	1217	PHE
1	C	1219	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42)

such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	140	GLN
1	A	204	GLN
1	A	331	ASN
1	A	353	ASN
1	A	371	ASN
1	A	384	ASN
1	A	413	ASN
1	A	440	ASN
1	A	630	GLN
1	A	789	GLN
1	A	876	HIS
1	A	938	GLN
1	A	984	GLN
1	A	1001	GLN
1	A	1091	GLN
1	A	1136	ASN
1	A	1180	GLN
1	B	73	ASN
1	B	160	HIS
1	B	204	GLN
1	B	248	ASN
1	B	587	ASN
1	B	605	ASN
1	B	630	GLN
1	B	872	ASN
1	B	998	ASN
1	B	1001	GLN
1	B	1091	GLN
1	B	1201	ASN
1	C	73	ASN
1	C	204	GLN
1	C	424	GLN
1	C	561	ASN
1	C	598	ASN
1	C	630	GLN
1	C	799	HIS
1	C	876	HIS
1	C	984	GLN
1	C	1001	GLN
1	C	1079	ASN
1	C	1126	ASN
1	C	1136	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

42 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	D	1	2,1	14,14,15	0.46	0	17,19,21	0.56	0
2	NAG	D	2	2	14,14,15	0.23	0	17,19,21	0.61	0
2	MAN	D	3	2	11,11,12	1.48	2 (18%)	15,15,17	1.61	3 (20%)
2	MAN	D	4	2	11,11,12	0.84	0	15,15,17	1.35	2 (13%)
2	MAN	D	5	2	11,11,12	1.22	2 (18%)	15,15,17	1.54	4 (26%)
2	MAN	D	6	2	11,11,12	0.77	0	15,15,17	1.20	1 (6%)
3	NAG	E	1	3,1	14,14,15	0.32	0	17,19,21	0.42	0
3	NAG	E	2	3	14,14,15	0.38	0	17,19,21	0.53	0
3	NAG	F	1	3,1	14,14,15	0.75	1 (7%)	17,19,21	0.74	0
3	NAG	F	2	3	14,14,15	0.38	0	17,19,21	0.68	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.24	0	17,19,21	0.82	1 (5%)
3	NAG	G	2	3	14,14,15	0.50	0	17,19,21	0.71	1 (5%)
3	NAG	H	1	3,1	14,14,15	0.34	0	17,19,21	0.79	1 (5%)
3	NAG	H	2	3	14,14,15	0.32	0	17,19,21	0.66	1 (5%)
2	NAG	I	1	2,1	14,14,15	0.34	0	17,19,21	0.63	1 (5%)
2	NAG	I	2	2	14,14,15	0.23	0	17,19,21	0.54	0
2	MAN	I	3	2	11,11,12	1.38	3 (27%)	15,15,17	1.80	3 (20%)
2	MAN	I	4	2	11,11,12	0.82	0	15,15,17	1.14	2 (13%)
2	MAN	I	5	2	11,11,12	0.80	0	15,15,17	1.05	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	I	6	2	11,11,12	0.73	0	15,15,17	1.27	2 (13%)
3	NAG	J	1	3,1	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	J	2	3	14,14,15	0.32	0	17,19,21	0.52	0
3	NAG	K	1	3,1	14,14,15	0.37	0	17,19,21	0.46	0
3	NAG	K	2	3	14,14,15	0.35	0	17,19,21	0.55	0
3	NAG	L	1	3,1	14,14,15	0.39	0	17,19,21	0.60	0
3	NAG	L	2	3	14,14,15	0.40	0	17,19,21	0.59	1 (5%)
3	NAG	M	1	3,1	14,14,15	0.22	0	17,19,21	0.49	0
3	NAG	M	2	3	14,14,15	0.39	0	17,19,21	0.50	0
2	NAG	N	1	2,1	14,14,15	0.39	0	17,19,21	0.47	0
2	NAG	N	2	2	14,14,15	0.25	0	17,19,21	0.70	0
2	MAN	N	3	2	11,11,12	1.20	1 (9%)	15,15,17	1.35	2 (13%)
2	MAN	N	4	2	11,11,12	0.97	1 (9%)	15,15,17	1.29	2 (13%)
2	MAN	N	5	2	11,11,12	0.75	0	15,15,17	1.09	2 (13%)
2	MAN	N	6	2	11,11,12	0.91	1 (9%)	15,15,17	1.54	2 (13%)
3	NAG	O	1	3,1	14,14,15	0.37	0	17,19,21	0.63	1 (5%)
3	NAG	O	2	3	14,14,15	0.30	0	17,19,21	0.50	0
3	NAG	P	1	3,1	14,14,15	0.24	0	17,19,21	0.64	0
3	NAG	P	2	3	14,14,15	0.46	0	17,19,21	0.76	1 (5%)
3	NAG	Q	1	3,1	14,14,15	0.34	0	17,19,21	0.52	0
3	NAG	Q	2	3	14,14,15	0.24	0	17,19,21	0.72	1 (5%)
3	NAG	R	1	3,1	14,14,15	0.19	0	17,19,21	0.48	0
3	NAG	R	2	3	14,14,15	0.27	0	17,19,21	0.45	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
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	MAN	D	3	2	-	2/2/19/22	1/1/1/1
2	MAN	D	4	2	-	1/2/19/22	0/1/1/1
2	MAN	D	5	2	-	2/2/19/22	0/1/1/1
2	MAN	D	6	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	MAN	I	3	2	-	2/2/19/22	1/1/1/1
2	MAN	I	4	2	-	2/2/19/22	0/1/1/1
2	MAN	I	5	2	-	0/2/19/22	0/1/1/1
2	MAN	I	6	2	-	2/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	1/6/23/26	0/1/1/1
2	MAN	N	3	2	-	2/2/19/22	1/1/1/1
2	MAN	N	4	2	-	2/2/19/22	0/1/1/1
2	MAN	N	5	2	-	2/2/19/22	0/1/1/1
2	MAN	N	6	2	-	2/2/19/22	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5	MAN	C1-C2	3.30	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	MAN	O5-C5	2.89	1.49	1.43
3	F	1	NAG	O5-C1	-2.61	1.39	1.43
2	I	3	MAN	O5-C5	2.59	1.48	1.43
2	D	3	MAN	C2-C3	2.44	1.56	1.52
2	N	3	MAN	O5-C5	2.40	1.48	1.43
2	I	3	MAN	C2-C3	2.39	1.56	1.52
2	N	6	MAN	O5-C5	2.14	1.47	1.43
2	I	3	MAN	C1-C2	2.05	1.56	1.52
2	N	4	MAN	O5-C5	2.03	1.47	1.43
2	D	5	MAN	C2-C3	2.02	1.55	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	3	MAN	C1-O5-C5	5.43	119.55	112.19
2	N	6	MAN	C1-O5-C5	4.97	118.92	112.19
2	D	3	MAN	C1-O5-C5	4.89	118.82	112.19
2	I	6	MAN	C1-O5-C5	3.83	117.38	112.19
2	N	3	MAN	C1-O5-C5	3.82	117.36	112.19
2	D	6	MAN	C1-O5-C5	3.50	116.93	112.19
2	N	4	MAN	C1-O5-C5	3.37	116.76	112.19
2	D	5	MAN	C1-O5-C5	3.18	116.50	112.19
2	I	4	MAN	C1-O5-C5	3.15	116.46	112.19
2	D	4	MAN	C1-O5-C5	3.11	116.40	112.19
2	D	5	MAN	C1-C2-C3	2.91	113.24	109.67
2	I	5	MAN	C1-O5-C5	2.79	115.97	112.19
3	P	2	NAG	C1-O5-C5	2.65	115.78	112.19
3	G	1	NAG	C1-O5-C5	2.64	115.77	112.19
3	Q	2	NAG	C1-O5-C5	2.55	115.65	112.19
2	I	3	MAN	C1-C2-C3	2.53	112.78	109.67
2	N	5	MAN	C1-O5-C5	2.50	115.58	112.19
3	G	2	NAG	C1-O5-C5	2.49	115.56	112.19
3	F	2	NAG	C1-O5-C5	2.42	115.47	112.19
2	N	6	MAN	O2-C2-C3	-2.42	105.30	110.14
3	H	2	NAG	C1-O5-C5	2.31	115.33	112.19
2	I	6	MAN	O2-C2-C3	-2.29	105.54	110.14
2	D	3	MAN	C1-C2-C3	2.24	112.42	109.67
2	I	3	MAN	O2-C2-C3	-2.23	105.68	110.14
2	D	5	MAN	O5-C1-C2	2.22	114.20	110.77
2	N	3	MAN	O2-C2-C3	-2.21	105.71	110.14
2	I	4	MAN	O2-C2-C3	-2.21	105.71	110.14
2	I	5	MAN	O2-C2-C3	-2.20	105.74	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	5	MAN	O2-C2-C3	-2.18	105.76	110.14
3	H	1	NAG	C1-O5-C5	2.15	115.11	112.19
2	D	4	MAN	C3-C4-C5	-2.14	106.43	110.24
2	N	4	MAN	C1-C2-C3	-2.07	107.12	109.67
3	L	2	NAG	C1-O5-C5	2.04	114.95	112.19
3	O	1	NAG	C1-O5-C5	2.03	114.94	112.19
2	I	1	NAG	C1-O5-C5	2.02	114.93	112.19
2	D	3	MAN	C2-C3-C4	2.00	114.36	110.89
2	D	5	MAN	O2-C2-C3	-2.00	106.13	110.14

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	3	MAN	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	N	6	MAN	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
2	N	3	MAN	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
2	N	4	MAN	O5-C5-C6-O6
2	N	5	MAN	C4-C5-C6-O6
2	N	6	MAN	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
2	I	4	MAN	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
2	N	4	MAN	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	N	5	MAN	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	6	MAN	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	D	3	MAN	C4-C5-C6-O6
2	D	6	MAN	O5-C5-C6-O6
2	D	3	MAN	O5-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	I	4	MAN	C4-C5-C6-O6
2	D	5	MAN	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6
2	I	6	MAN	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	I	6	MAN	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
2	I	3	MAN	O5-C5-C6-O6
2	I	3	MAN	C4-C5-C6-O6

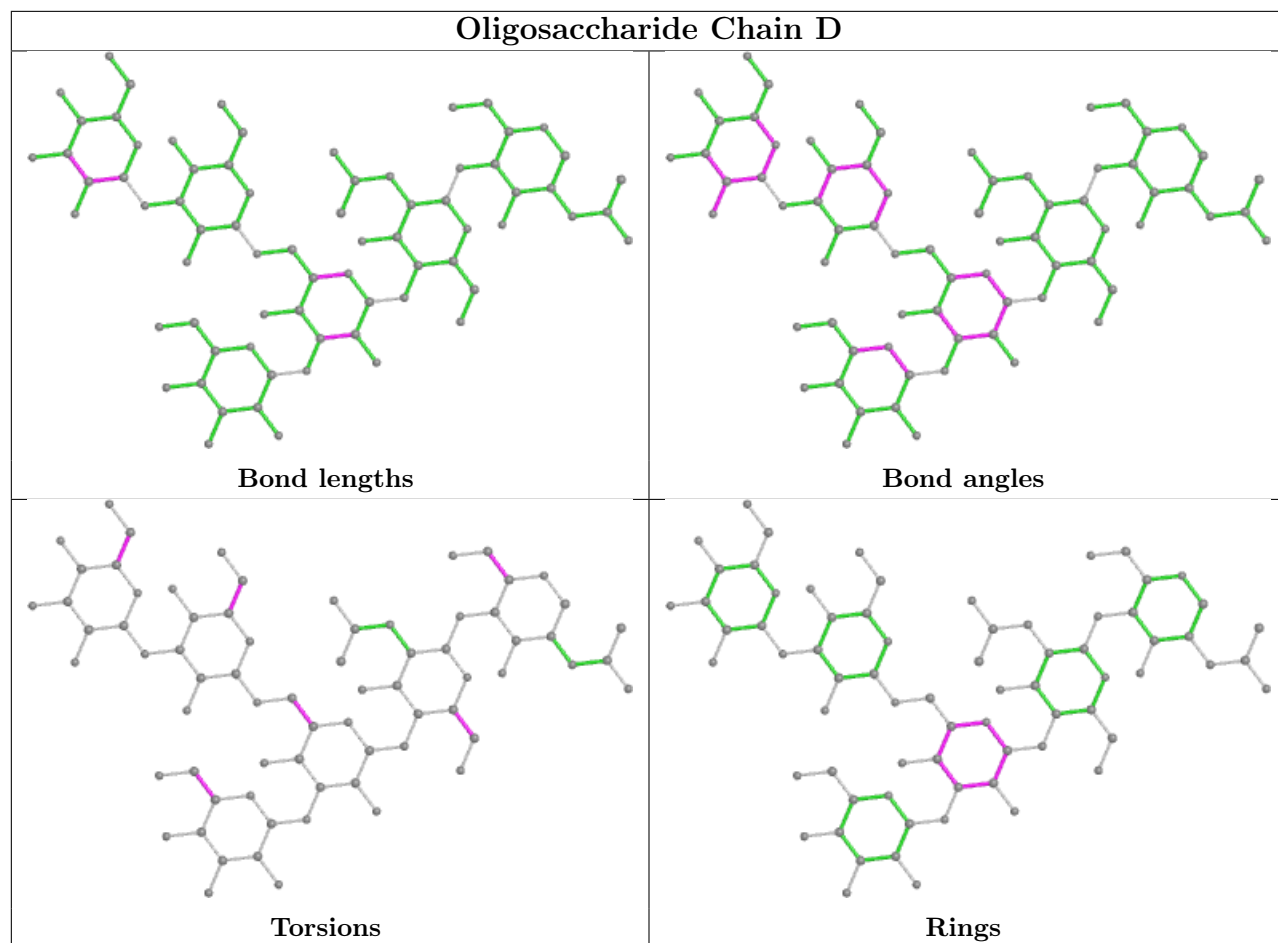
All (3) ring outliers are listed below:

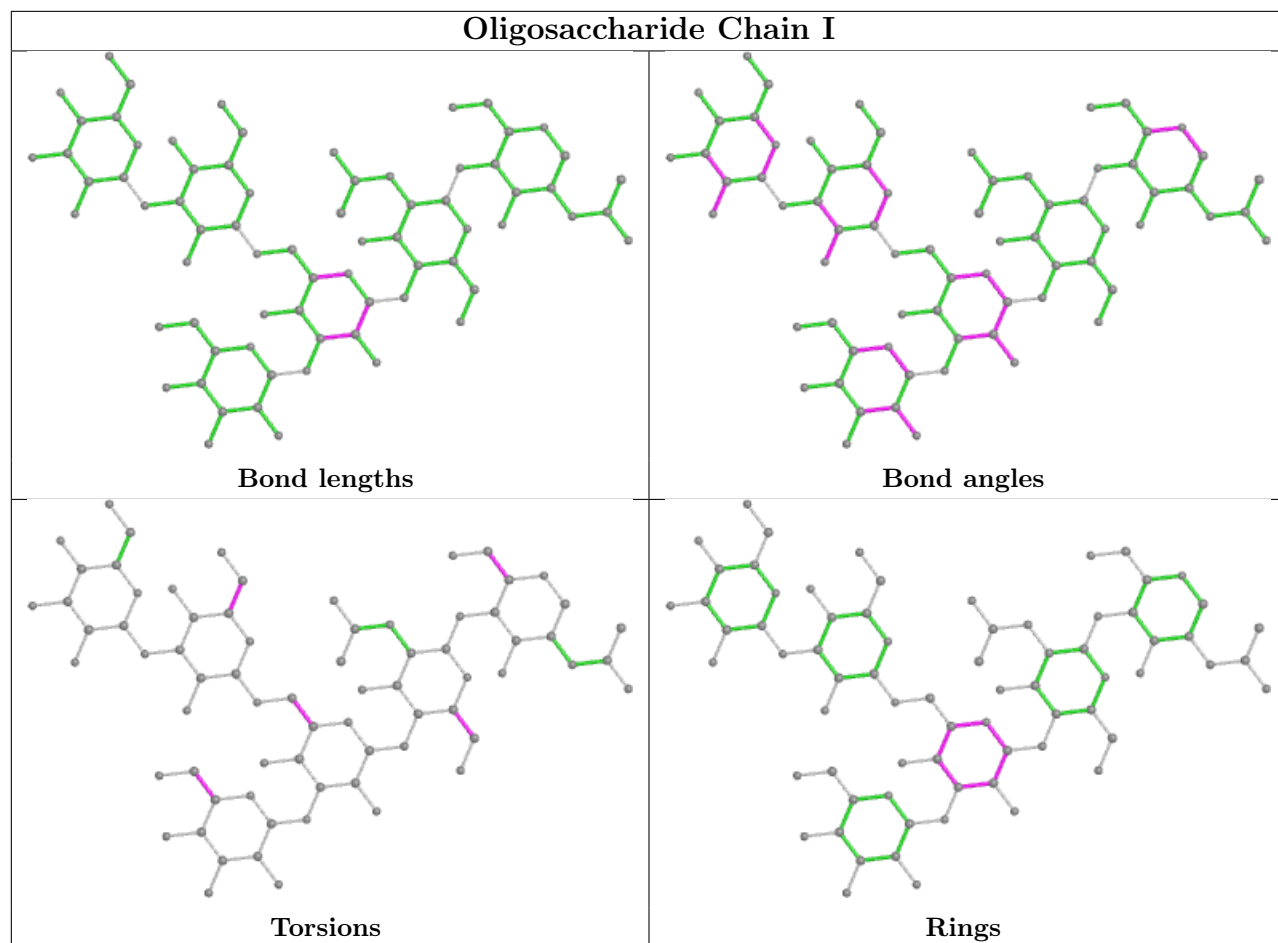
Mol	Chain	Res	Type	Atoms
2	I	3	MAN	C1-C2-C3-C4-C5-O5
2	D	3	MAN	C1-C2-C3-C4-C5-O5
2	N	3	MAN	C1-C2-C3-C4-C5-O5

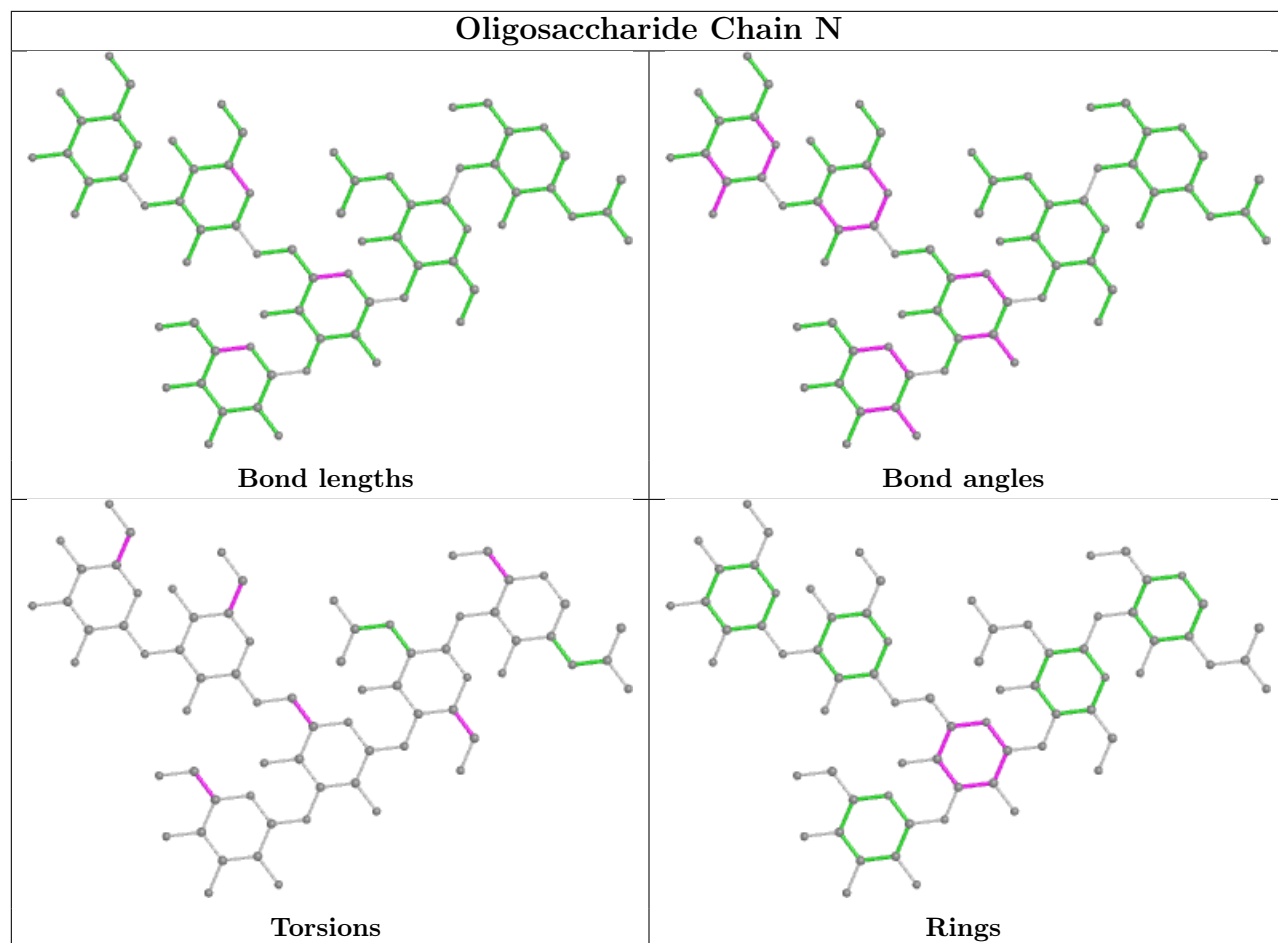
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0

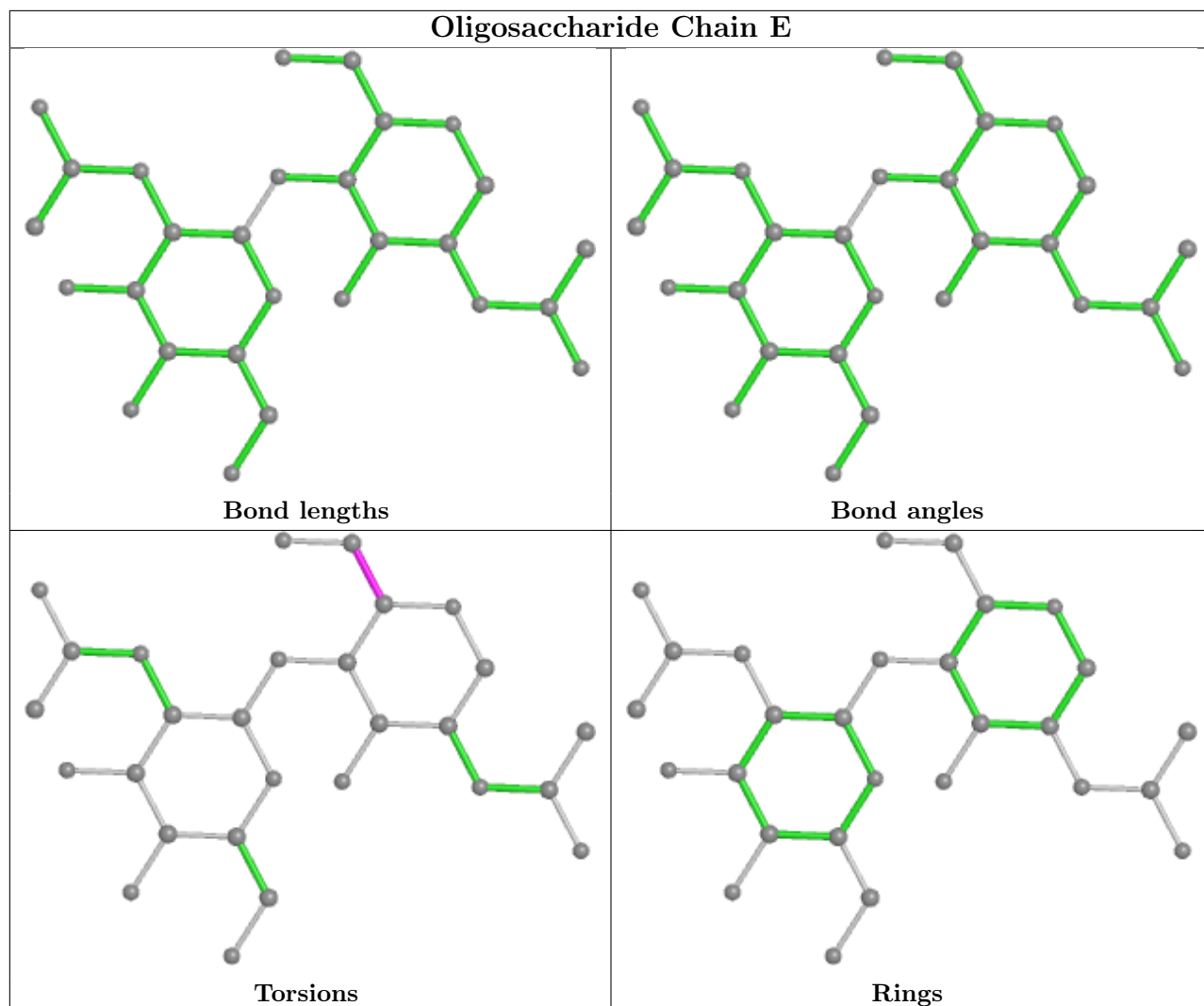
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

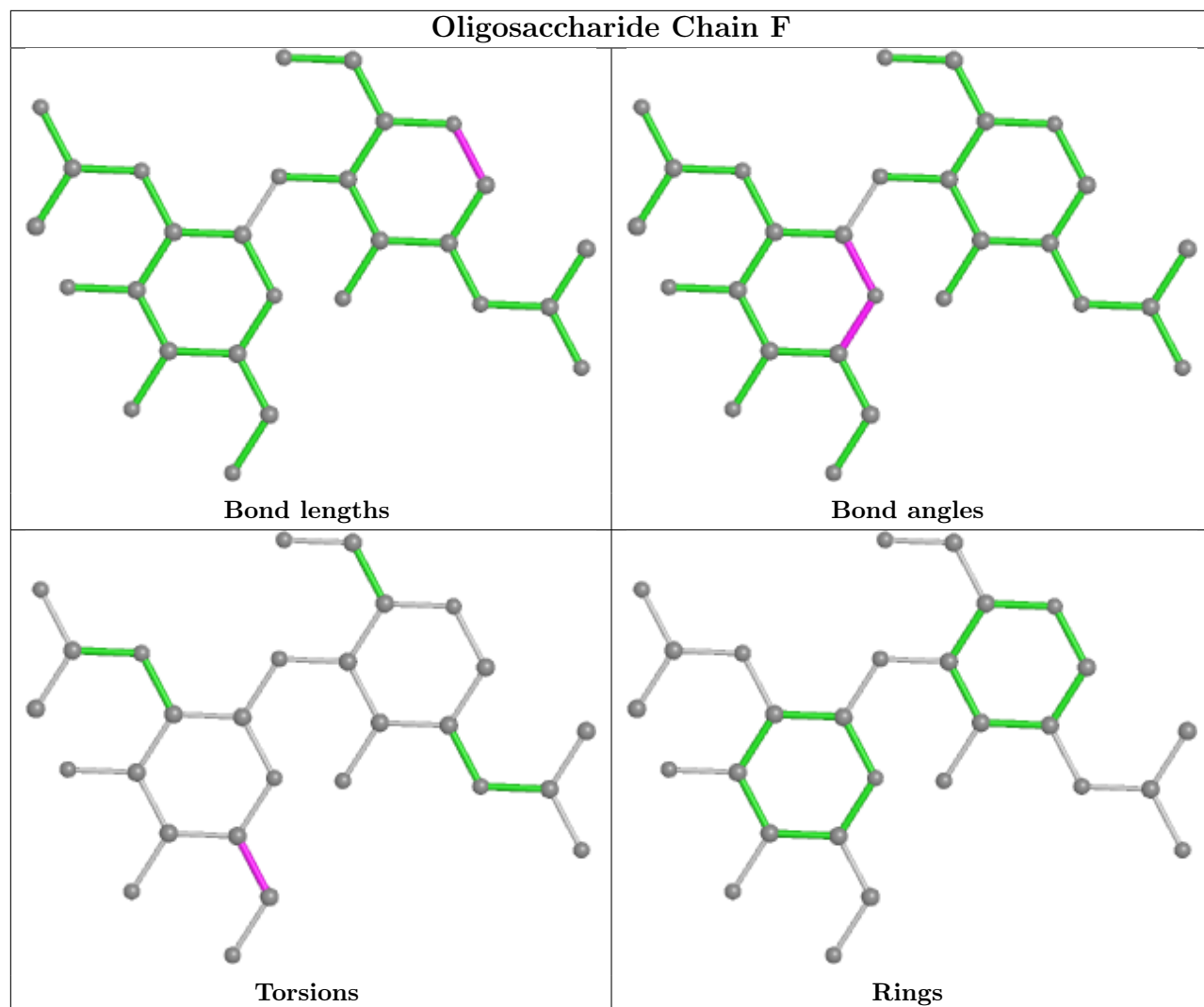


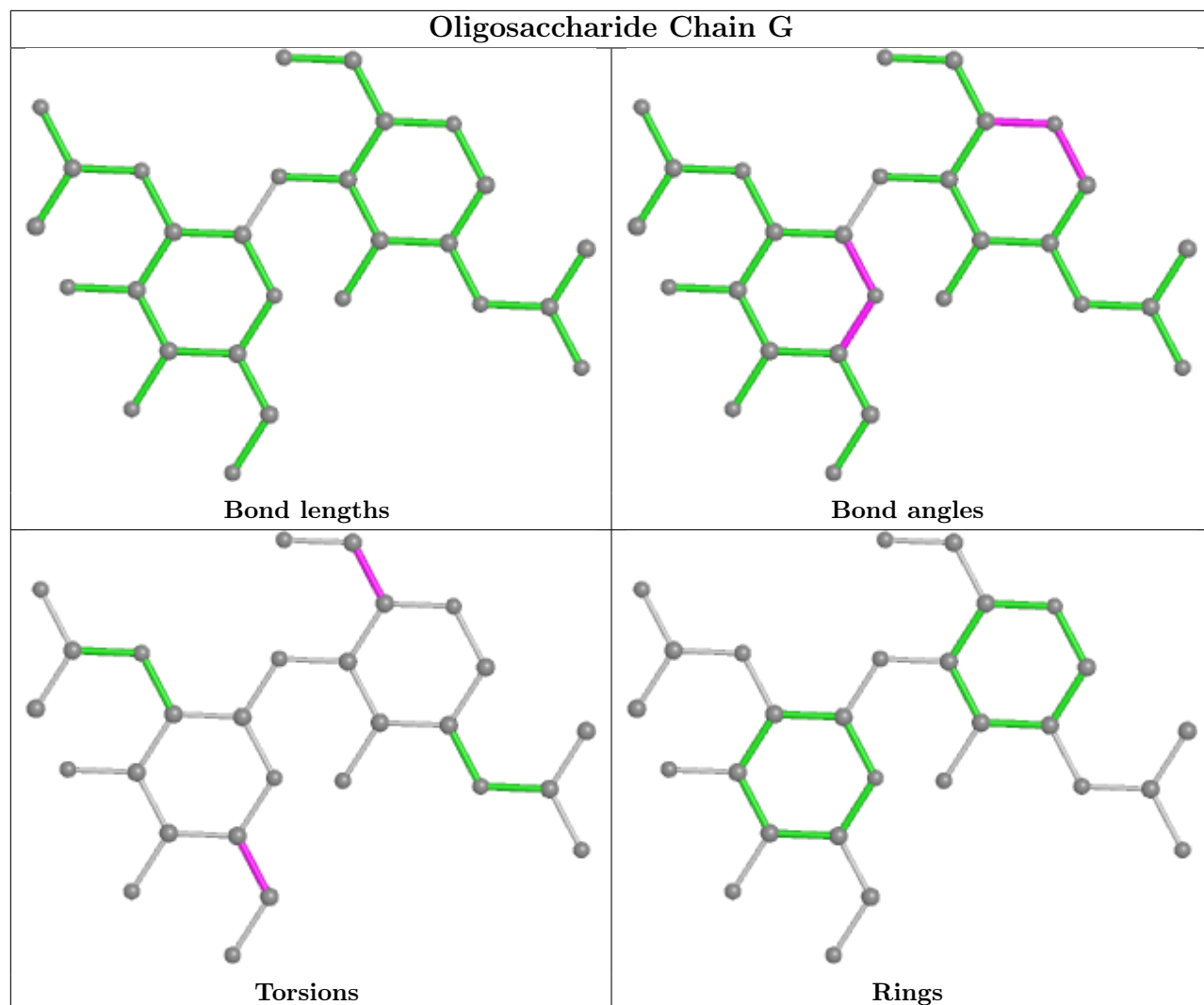


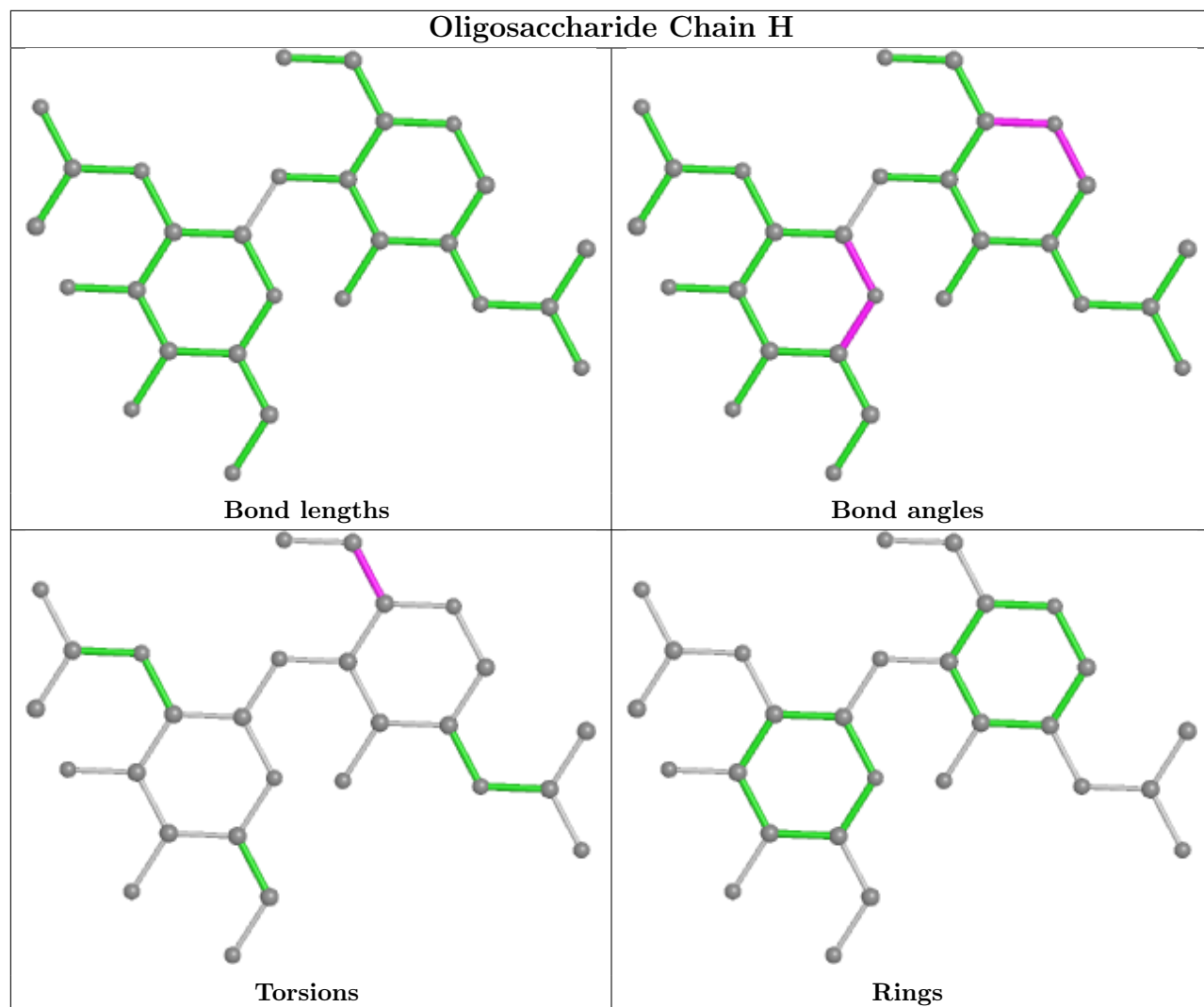


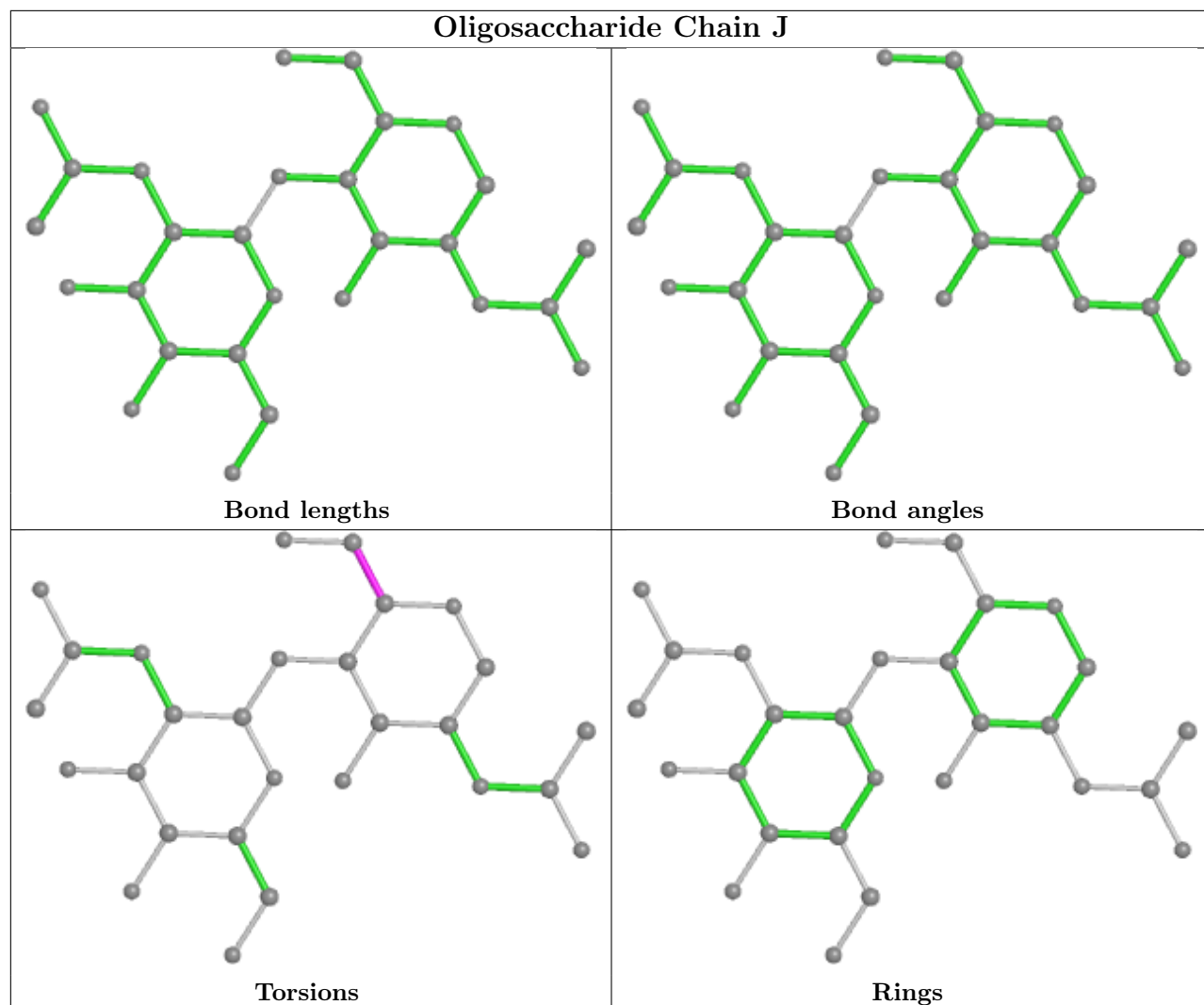


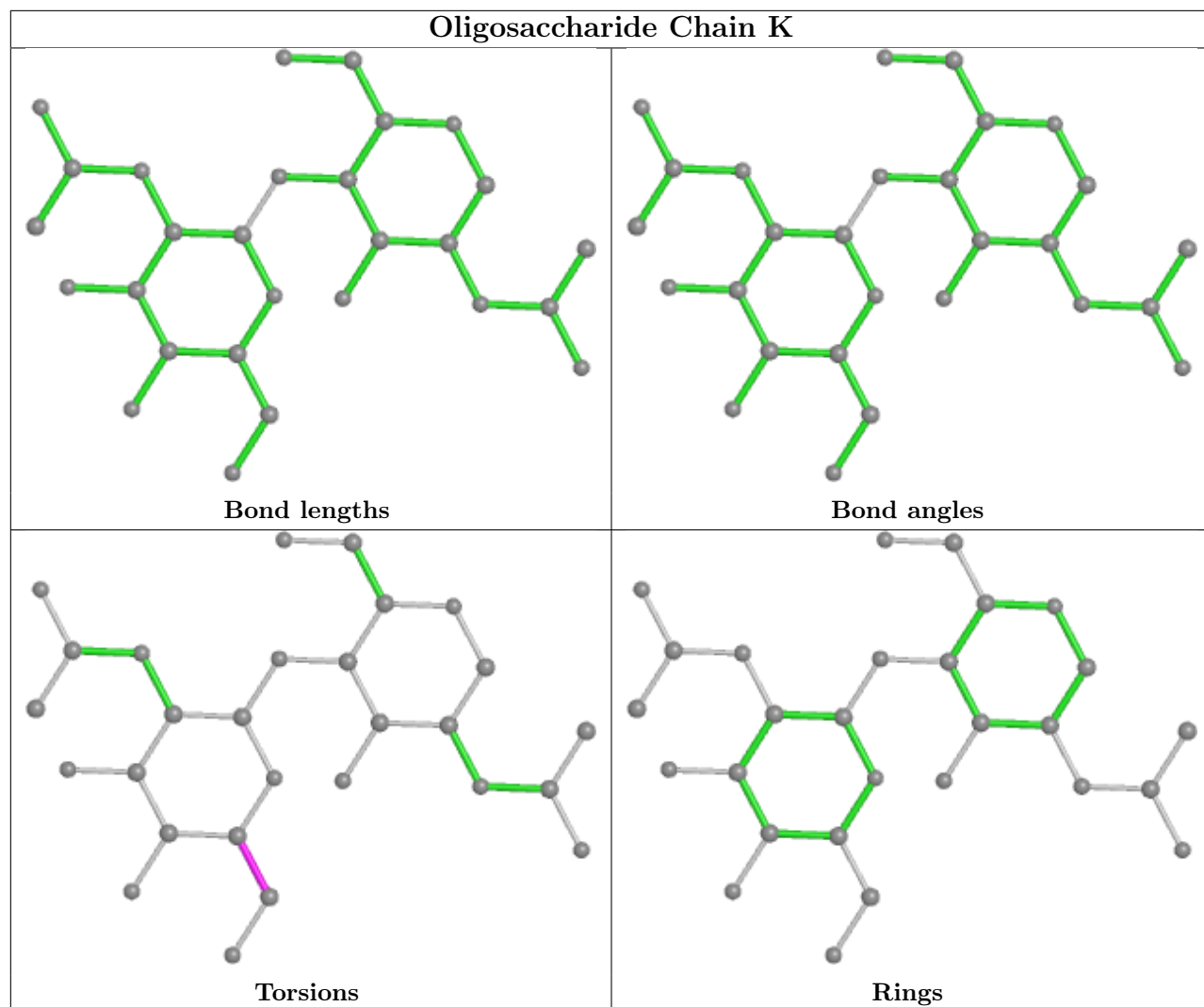


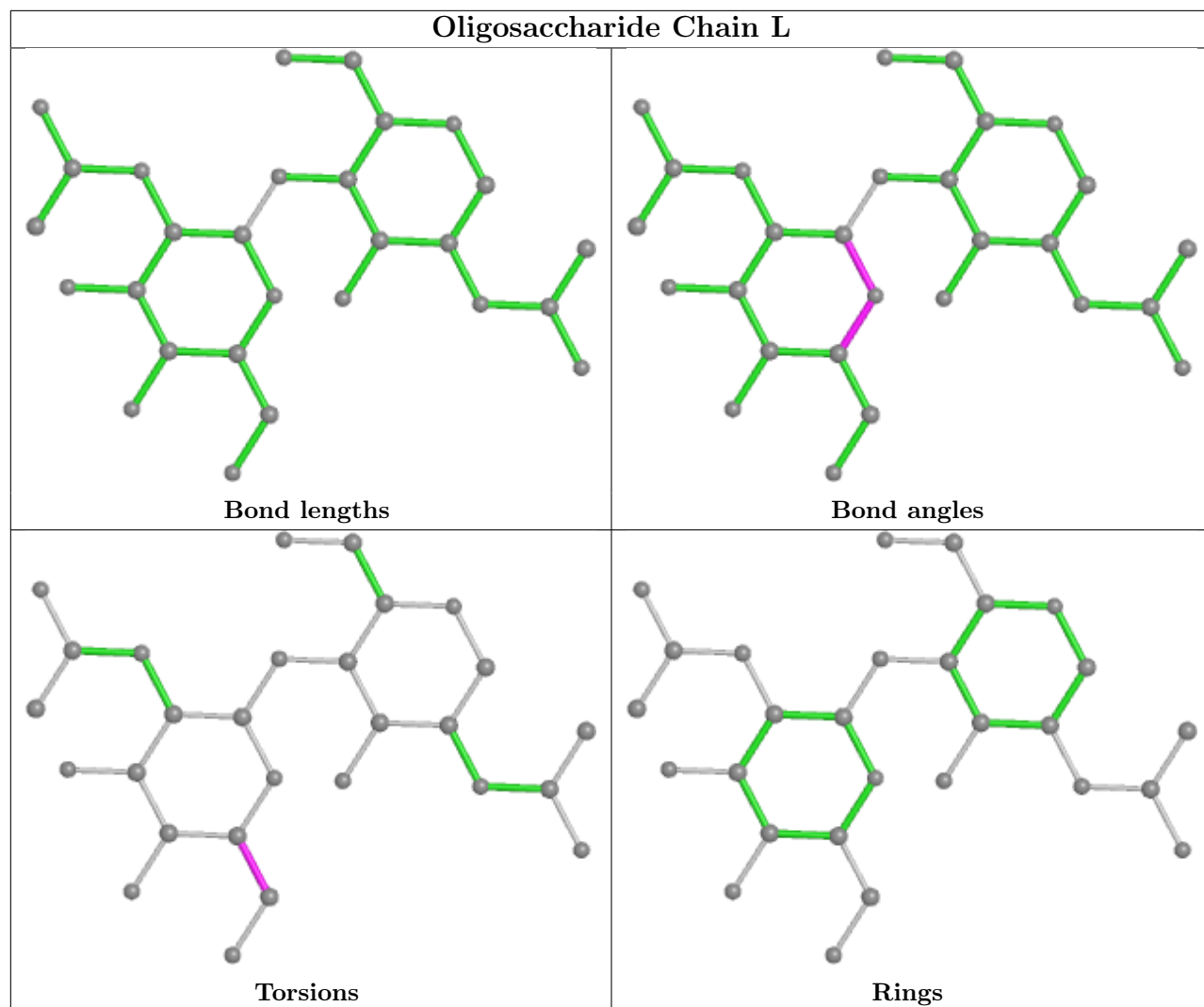


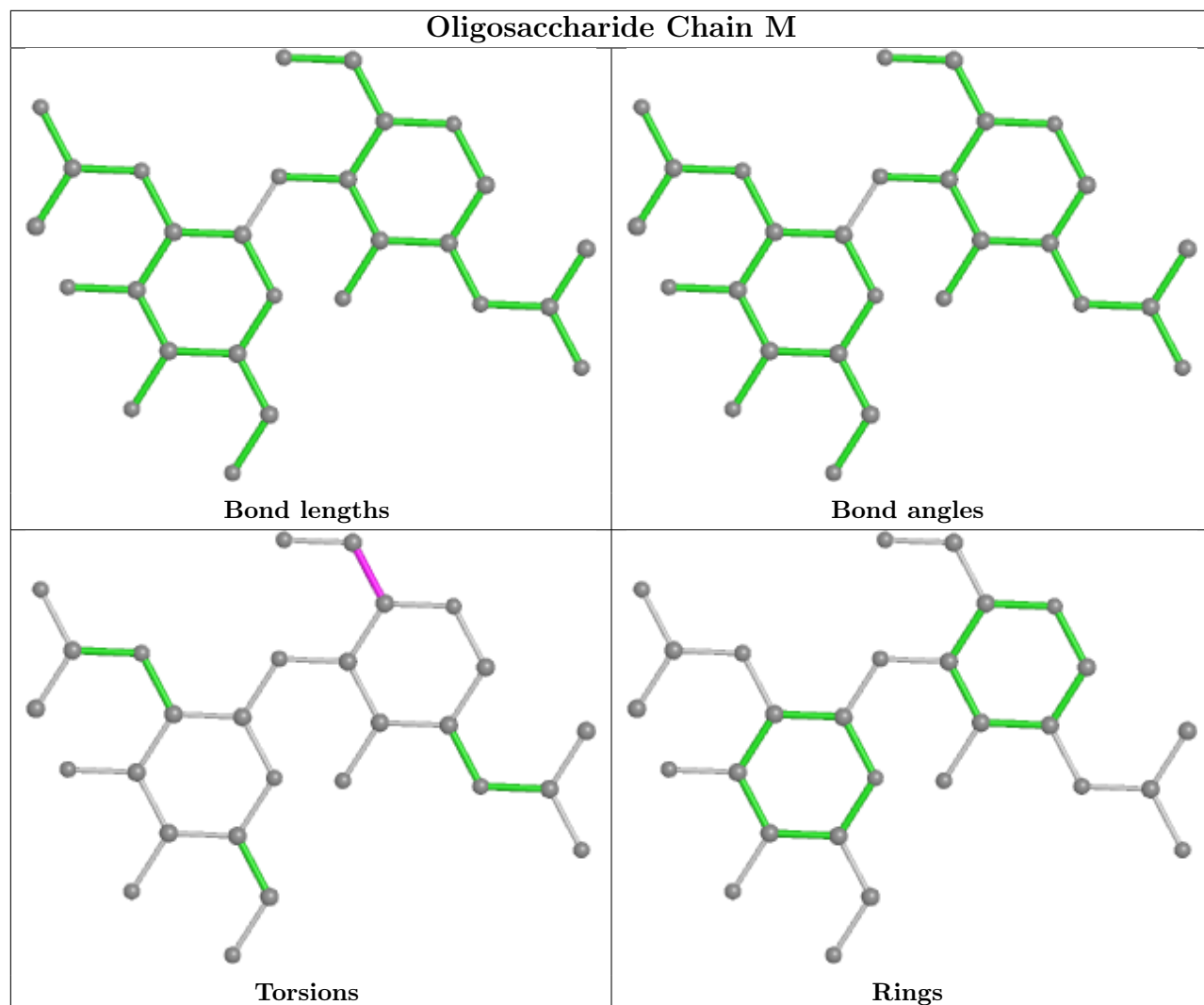




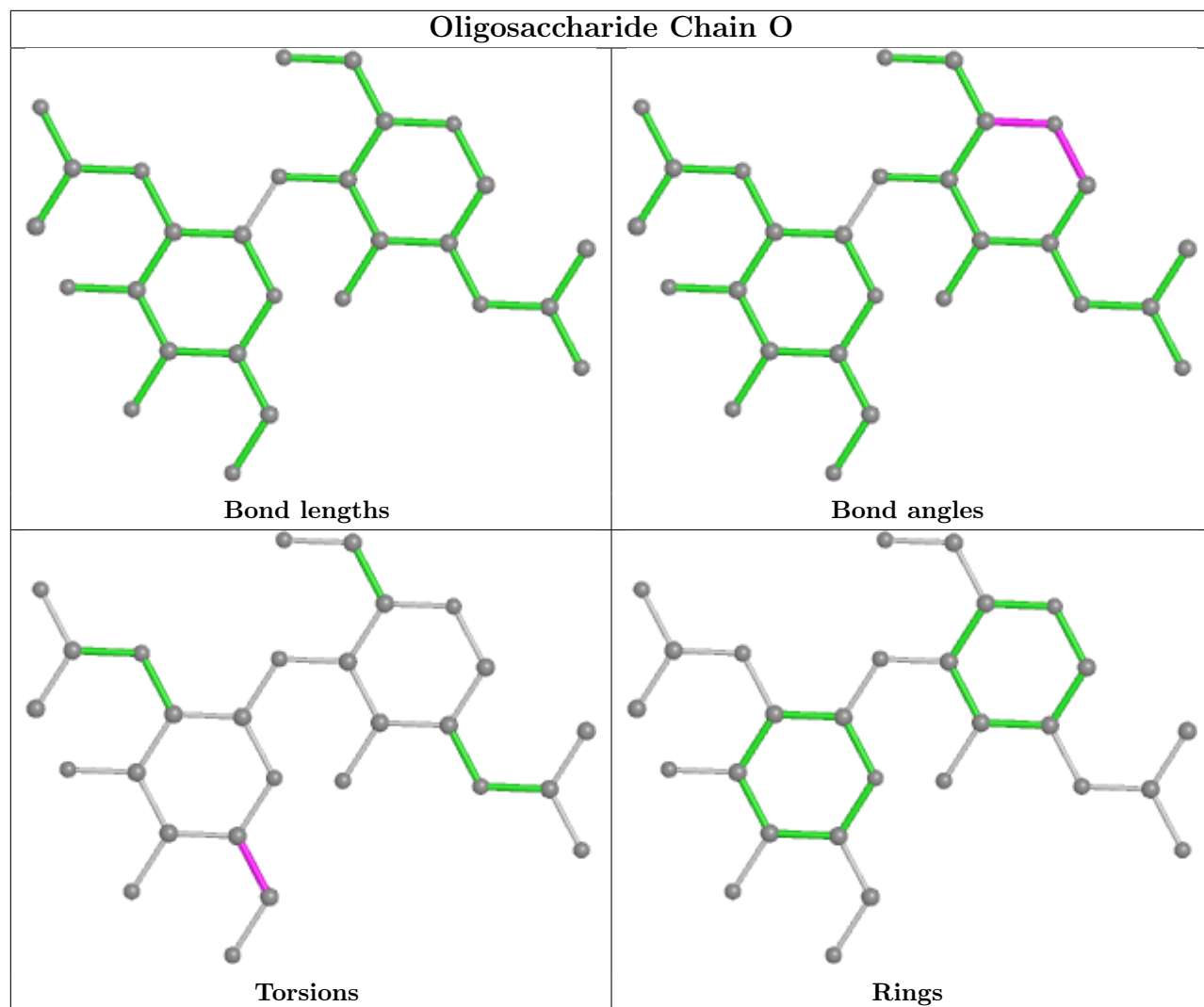


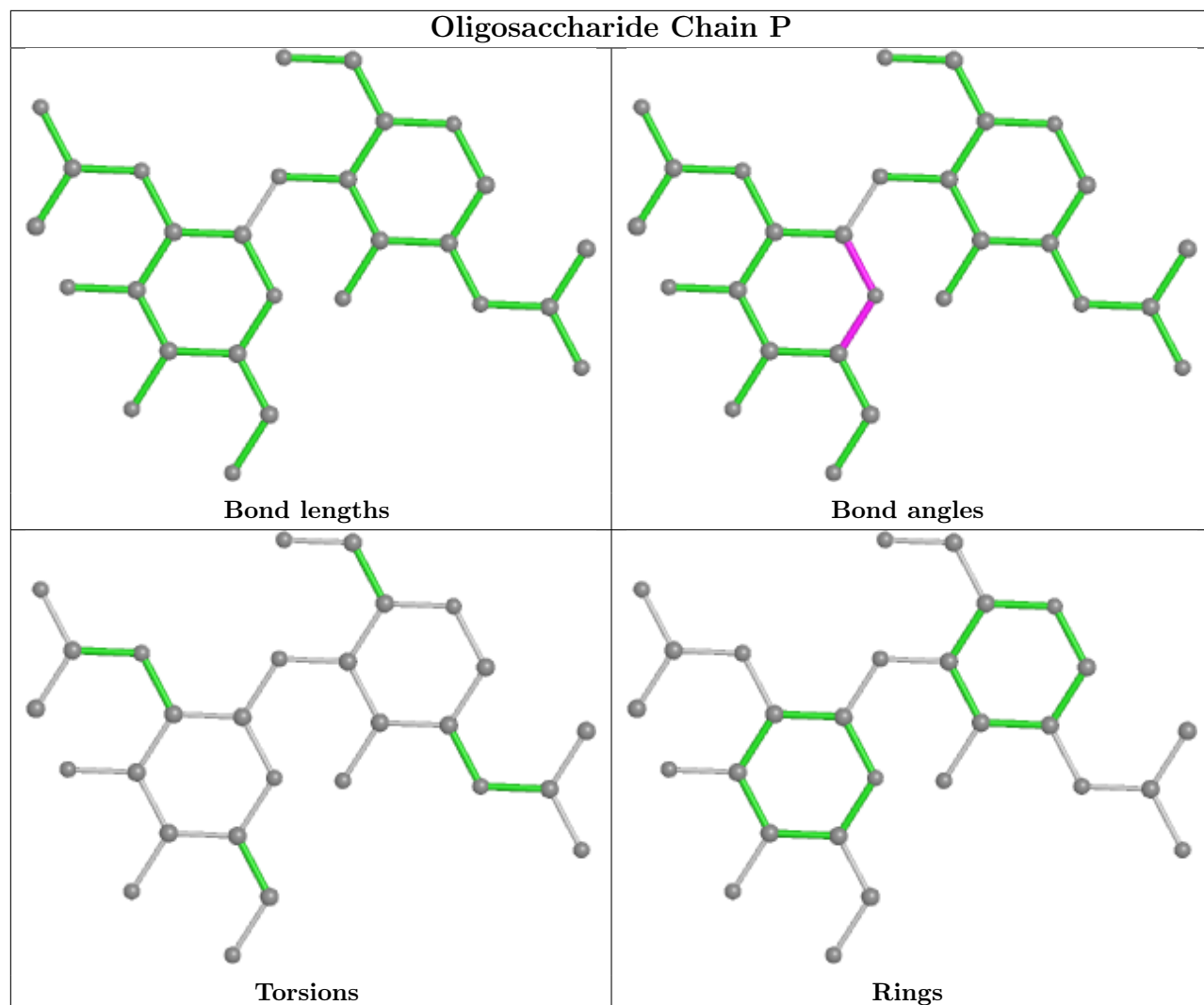


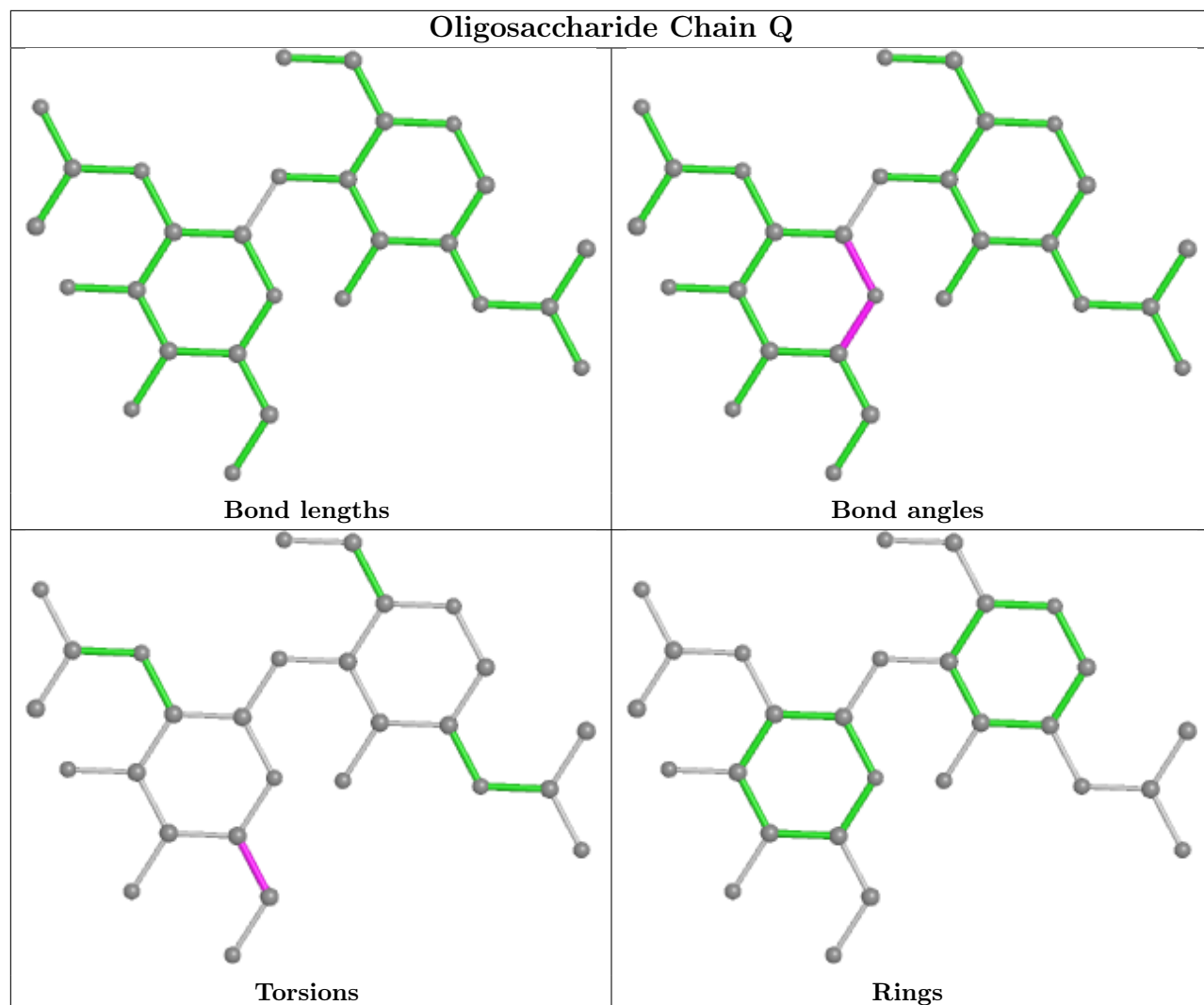


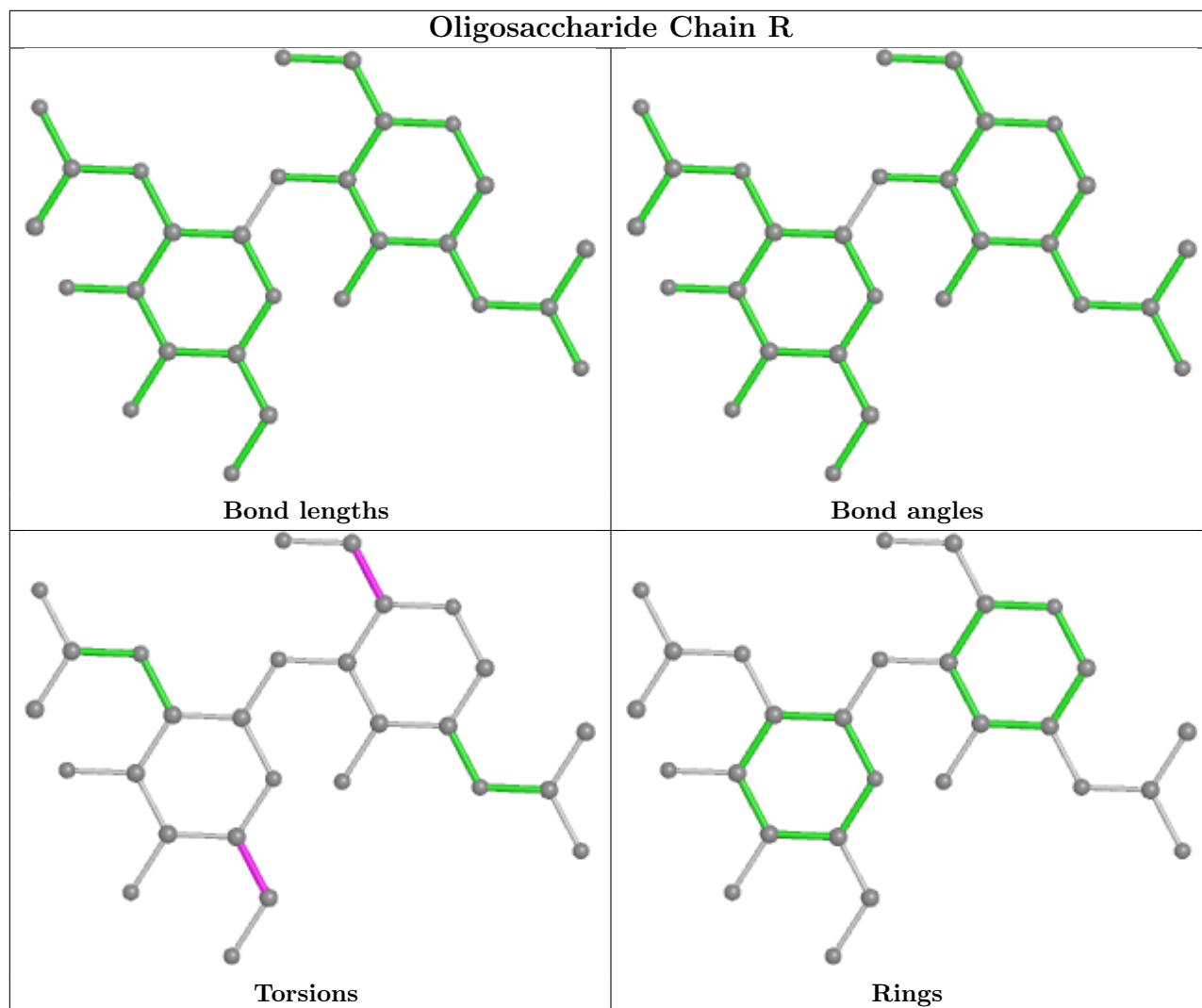












## 5.6 Ligand geometry [i](#)

51 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	A	2012	1	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
4	NAG	A	2011	1	14,14,15	0.21	0	17,19,21	0.54	0
4	NAG	B	2004	1	14,14,15	0.35	0	17,19,21	0.58	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	2005	1	14,14,15	0.28	0	17,19,21	0.48	0
4	NAG	C	2012	1	14,14,15	0.20	0	17,19,21	0.68	1 (5%)
4	NAG	B	2015	1	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
4	NAG	A	2003	1	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	A	2010	1	14,14,15	0.40	0	17,19,21	0.40	0
4	NAG	B	2005	1	14,14,15	0.36	0	17,19,21	0.52	0
4	NAG	A	2009	1	14,14,15	0.55	0	17,19,21	0.62	1 (5%)
4	NAG	C	2014	1	14,14,15	0.42	0	17,19,21	0.42	0
4	NAG	C	2004	1	14,14,15	0.27	0	17,19,21	0.48	0
4	NAG	C	2017	1	14,14,15	0.21	0	17,19,21	0.51	0
4	NAG	A	2006	1	14,14,15	0.23	0	17,19,21	0.62	1 (5%)
4	NAG	B	2017	1	14,14,15	0.49	0	17,19,21	0.66	1 (5%)
4	NAG	B	2009	1	14,14,15	0.36	0	17,19,21	0.72	1 (5%)
4	NAG	A	2015	1	14,14,15	0.23	0	17,19,21	0.59	0
4	NAG	B	2013	1	14,14,15	0.54	0	17,19,21	0.42	0
4	NAG	C	2002	1	14,14,15	0.65	0	17,19,21	0.65	1 (5%)
4	NAG	A	2005	1	14,14,15	0.28	0	17,19,21	0.70	0
4	NAG	C	2011	1	14,14,15	0.25	0	17,19,21	0.68	1 (5%)
4	NAG	B	2006	1	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	B	2016	1	14,14,15	0.32	0	17,19,21	0.57	0
4	NAG	A	2008	1	14,14,15	0.30	0	17,19,21	0.49	0
4	NAG	C	2016	1	14,14,15	0.37	0	17,19,21	0.47	0
4	NAG	B	2010	1	14,14,15	0.28	0	17,19,21	0.36	0
4	NAG	C	2008	1	14,14,15	0.19	0	17,19,21	0.63	1 (5%)
4	NAG	B	2012	1	14,14,15	0.31	0	17,19,21	0.76	1 (5%)
4	NAG	B	2008	1	14,14,15	0.43	0	17,19,21	0.53	0
4	NAG	C	2015	1	14,14,15	0.33	0	17,19,21	0.53	0
4	NAG	C	2001	1	14,14,15	0.60	0	17,19,21	0.70	1 (5%)
4	NAG	C	2007	1	14,14,15	0.42	0	17,19,21	0.46	0
4	NAG	C	2003	1	14,14,15	0.31	0	17,19,21	0.36	0
4	NAG	A	2007	1	14,14,15	0.52	0	17,19,21	0.70	1 (5%)
4	NAG	B	2011	1	14,14,15	0.28	0	17,19,21	0.51	0
4	NAG	A	2001	1	14,14,15	0.53	0	17,19,21	0.60	1 (5%)
4	NAG	B	2007	1	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	C	2009	1	14,14,15	0.36	0	17,19,21	0.52	0
4	NAG	A	2002	1	14,14,15	0.50	0	17,19,21	0.57	0
4	NAG	A	2004	1	14,14,15	0.47	0	17,19,21	0.45	0
4	NAG	A	2016	1	14,14,15	0.36	0	17,19,21	0.62	1 (5%)
4	NAG	A	2017	1	14,14,15	0.39	0	17,19,21	0.67	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	2002	1	14,14,15	0.50	0	17,19,21	0.67	1 (5%)
4	NAG	B	2003	1	14,14,15	0.28	0	17,19,21	0.42	0
4	NAG	B	2014	1	14,14,15	0.54	0	17,19,21	0.40	0
4	NAG	C	2006	1	14,14,15	0.39	0	17,19,21	0.60	1 (5%)
4	NAG	C	2010	1	14,14,15	0.51	0	17,19,21	0.39	0
4	NAG	B	2001	1	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
4	NAG	A	2014	1	14,14,15	0.54	0	17,19,21	0.78	1 (5%)
4	NAG	C	2013	1	14,14,15	0.39	0	17,19,21	0.41	0
4	NAG	A	2013	1	14,14,15	0.45	0	17,19,21	0.60	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	A	2012	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2011	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2012	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2015	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2010	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2005	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2009	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2014	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2017	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2017	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2015	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2013	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2011	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2006	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	2016	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2008	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2016	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2010	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2012	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2015	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2007	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2011	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2016	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2017	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2014	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2006	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2010	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2013	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2013	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2014	NAG	C1-O5-C5	2.96	116.20	112.19
4	B	2015	NAG	C1-O5-C5	2.91	116.14	112.19
4	B	2012	NAG	C1-O5-C5	2.69	115.83	112.19
4	B	2009	NAG	C1-O5-C5	2.47	115.53	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2001	NAG	C1-O5-C5	2.44	115.49	112.19
4	B	2002	NAG	C1-O5-C5	2.38	115.41	112.19
4	C	2002	NAG	C1-O5-C5	2.35	115.38	112.19
4	C	2011	NAG	C1-O5-C5	2.35	115.38	112.19
4	A	2007	NAG	C1-O5-C5	2.34	115.37	112.19
4	C	2012	NAG	C1-O5-C5	2.32	115.33	112.19
4	B	2001	NAG	C8-C7-N2	2.31	120.01	116.10
4	B	2017	NAG	C1-O5-C5	2.30	115.31	112.19
4	A	2012	NAG	C1-O5-C5	2.26	115.25	112.19
4	A	2017	NAG	C1-O5-C5	2.20	115.18	112.19
4	A	2009	NAG	C1-O5-C5	2.11	115.06	112.19
4	C	2008	NAG	C1-O5-C5	2.08	115.02	112.19
4	A	2001	NAG	C1-O5-C5	2.07	115.00	112.19
4	B	2001	NAG	C2-N2-C7	-2.04	119.99	122.90
4	C	2006	NAG	C1-O5-C5	2.03	114.94	112.19
4	A	2006	NAG	C1-O5-C5	2.02	114.93	112.19
4	A	2016	NAG	C1-O5-C5	2.01	114.92	112.19
4	B	2004	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2017	NAG	C4-C5-C6-O6
4	C	2004	NAG	O5-C5-C6-O6
4	A	2016	NAG	O5-C5-C6-O6
4	C	2003	NAG	O5-C5-C6-O6
4	C	2010	NAG	O5-C5-C6-O6
4	B	2010	NAG	O5-C5-C6-O6
4	C	2005	NAG	O5-C5-C6-O6
4	B	2007	NAG	C4-C5-C6-O6
4	A	2011	NAG	O5-C5-C6-O6
4	B	2009	NAG	O5-C5-C6-O6
4	B	2012	NAG	O5-C5-C6-O6
4	B	2015	NAG	O5-C5-C6-O6
4	C	2001	NAG	O5-C5-C6-O6
4	A	2016	NAG	C4-C5-C6-O6
4	B	2003	NAG	C4-C5-C6-O6
4	B	2017	NAG	O5-C5-C6-O6
4	A	2010	NAG	C4-C5-C6-O6
4	A	2006	NAG	O5-C5-C6-O6
4	B	2013	NAG	O5-C5-C6-O6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
4	C	2003	NAG	C4-C5-C6-O6
4	A	2013	NAG	O5-C5-C6-O6
4	B	2010	NAG	C4-C5-C6-O6
4	C	2004	NAG	C4-C5-C6-O6
4	A	2007	NAG	O5-C5-C6-O6
4	B	2011	NAG	O5-C5-C6-O6
4	C	2010	NAG	C4-C5-C6-O6
4	A	2010	NAG	O5-C5-C6-O6
4	B	2007	NAG	O5-C5-C6-O6
4	B	2013	NAG	C4-C5-C6-O6
4	A	2014	NAG	O5-C5-C6-O6
4	B	2003	NAG	O5-C5-C6-O6
4	B	2011	NAG	C4-C5-C6-O6
4	C	2001	NAG	C4-C5-C6-O6
4	C	2005	NAG	C4-C5-C6-O6
4	A	2006	NAG	C4-C5-C6-O6
4	B	2009	NAG	C4-C5-C6-O6
4	A	2011	NAG	C4-C5-C6-O6
4	A	2014	NAG	C4-C5-C6-O6
4	B	2012	NAG	C4-C5-C6-O6
4	B	2015	NAG	C4-C5-C6-O6
4	C	2008	NAG	O5-C5-C6-O6
4	C	2011	NAG	C4-C5-C6-O6
4	A	2007	NAG	C4-C5-C6-O6
4	A	2003	NAG	O5-C5-C6-O6
4	A	2005	NAG	O5-C5-C6-O6
4	C	2009	NAG	O5-C5-C6-O6
4	A	2005	NAG	C4-C5-C6-O6
4	C	2009	NAG	C4-C5-C6-O6
4	C	2011	NAG	O5-C5-C6-O6
4	A	2008	NAG	O5-C5-C6-O6
4	C	2008	NAG	C4-C5-C6-O6
4	B	2008	NAG	C4-C5-C6-O6
4	C	2007	NAG	O5-C5-C6-O6
4	C	2013	NAG	O5-C5-C6-O6
4	B	2014	NAG	O5-C5-C6-O6
4	C	2012	NAG	C4-C5-C6-O6
4	A	2013	NAG	C4-C5-C6-O6
4	C	2012	NAG	O5-C5-C6-O6
4	B	2008	NAG	O5-C5-C6-O6
4	A	2015	NAG	C4-C5-C6-O6
4	A	2015	NAG	O5-C5-C6-O6

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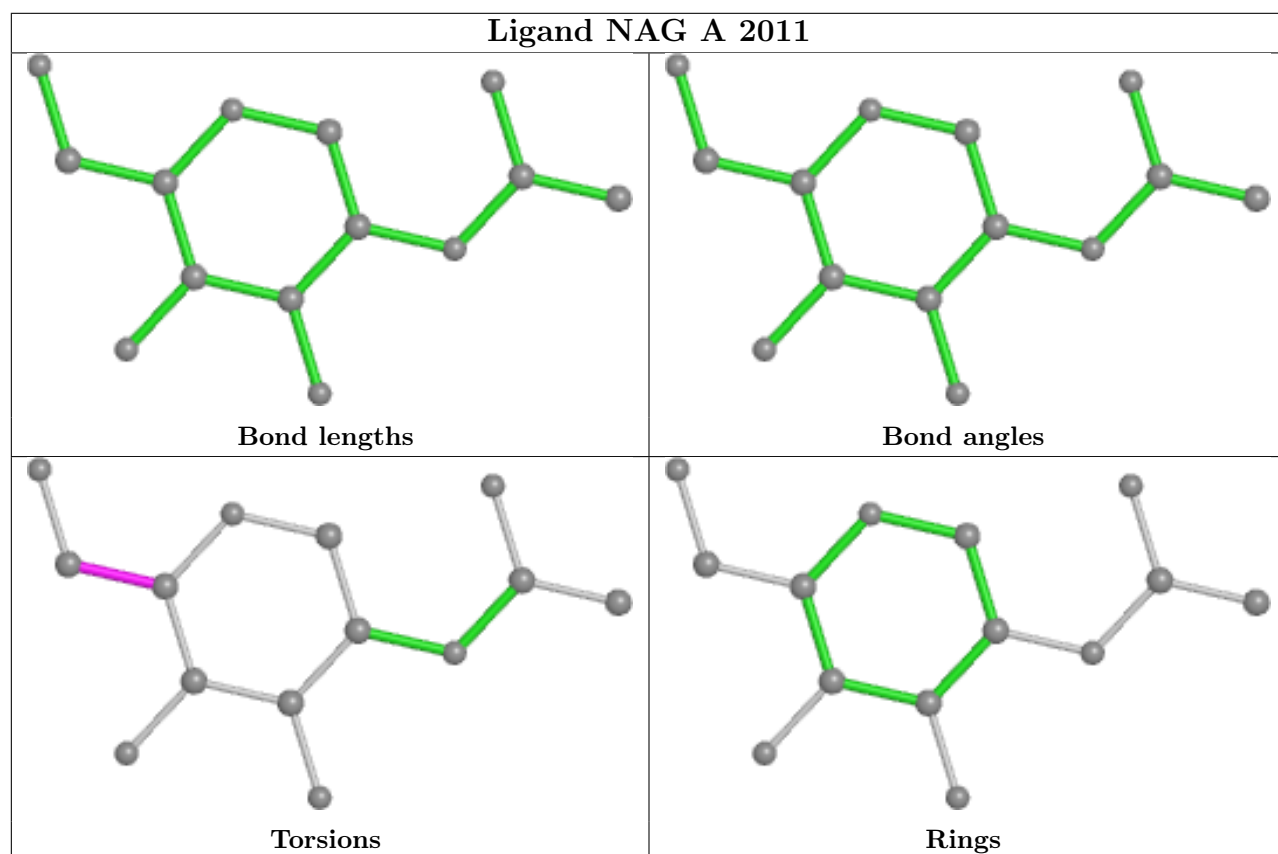
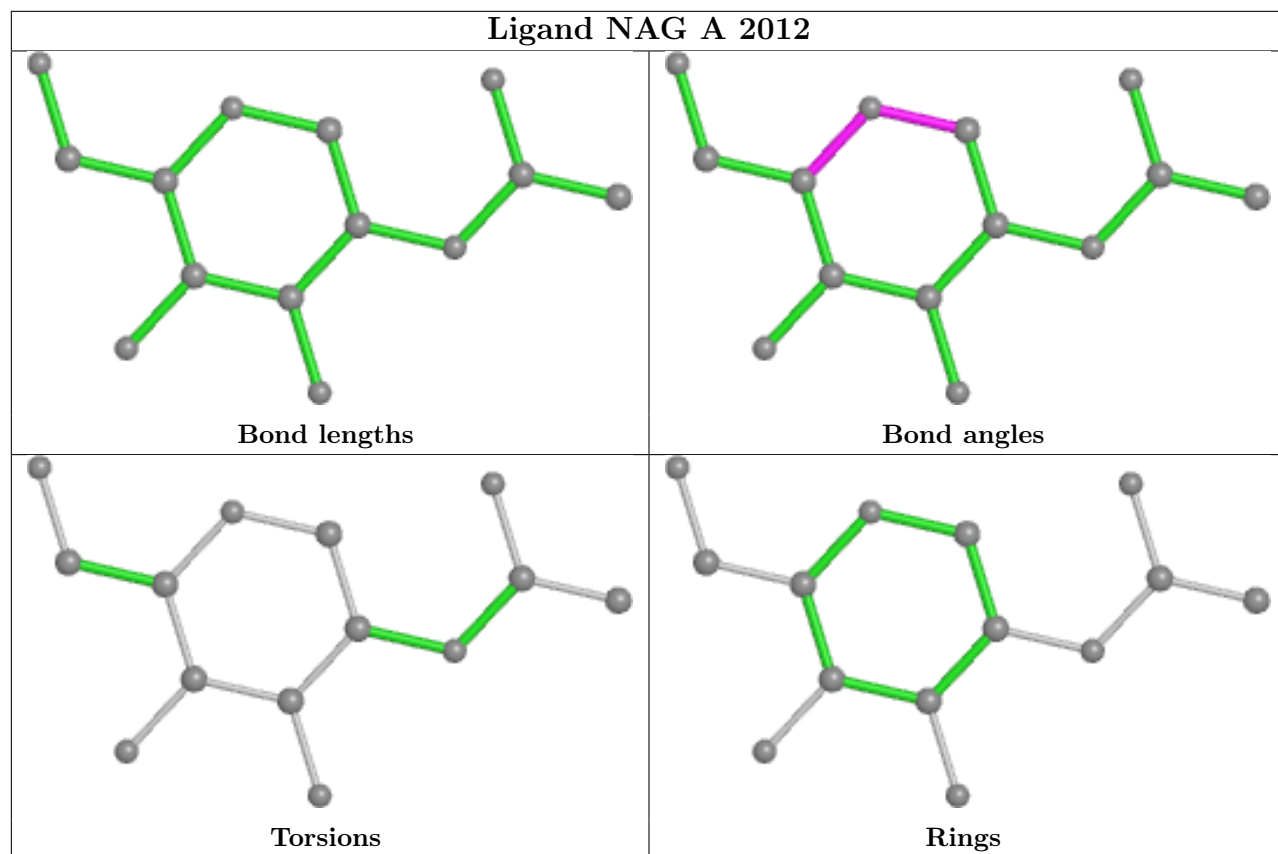
Mol	Chain	Res	Type	Atoms
4	C	2014	NAG	O5-C5-C6-O6
4	A	2003	NAG	C4-C5-C6-O6

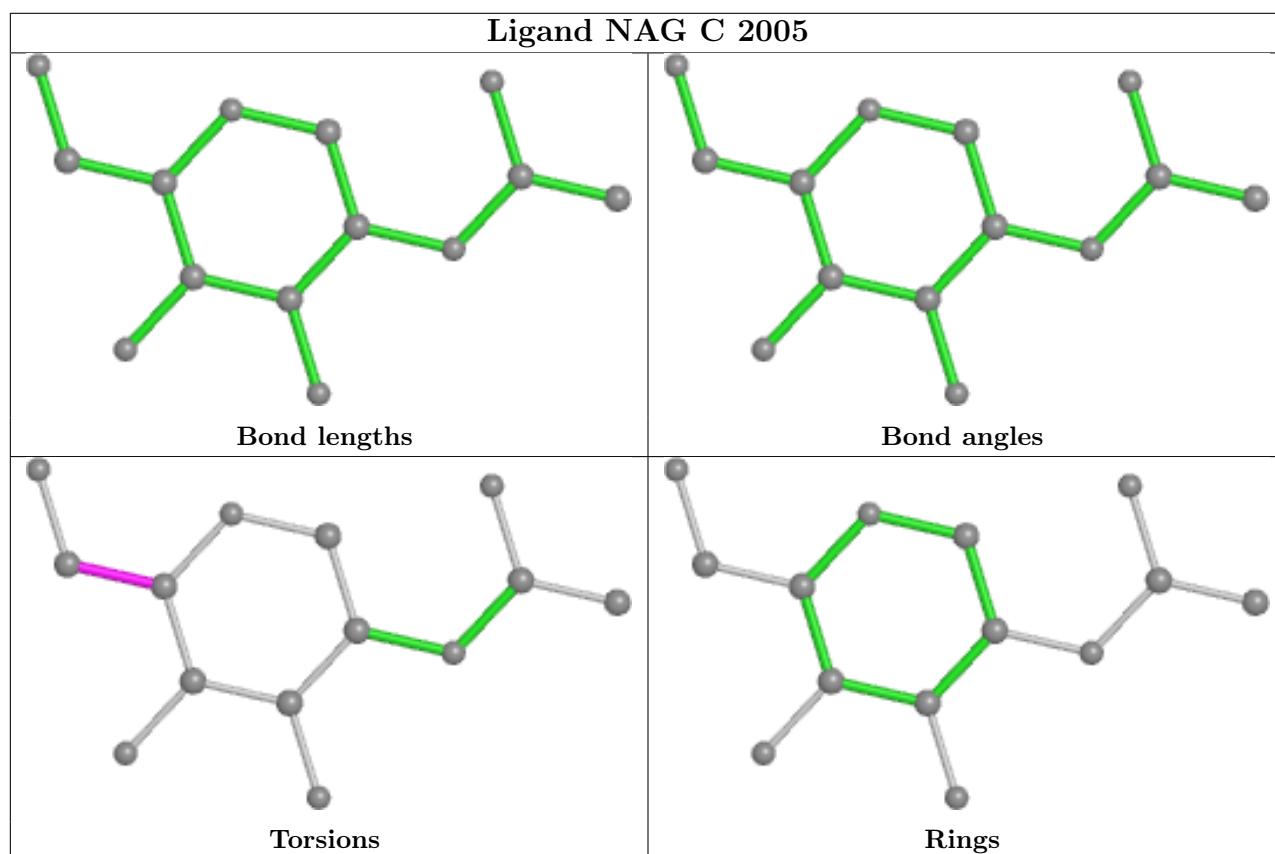
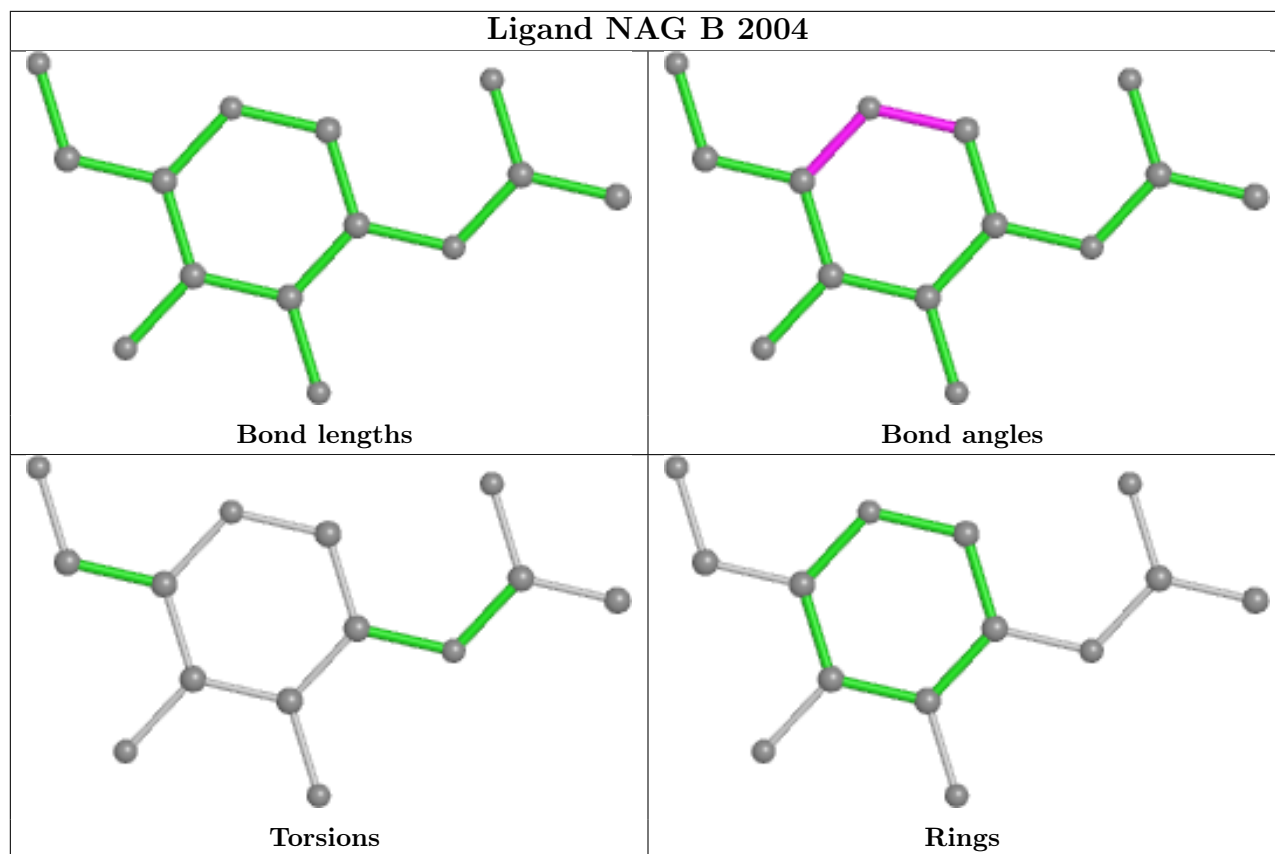
There are no ring outliers.

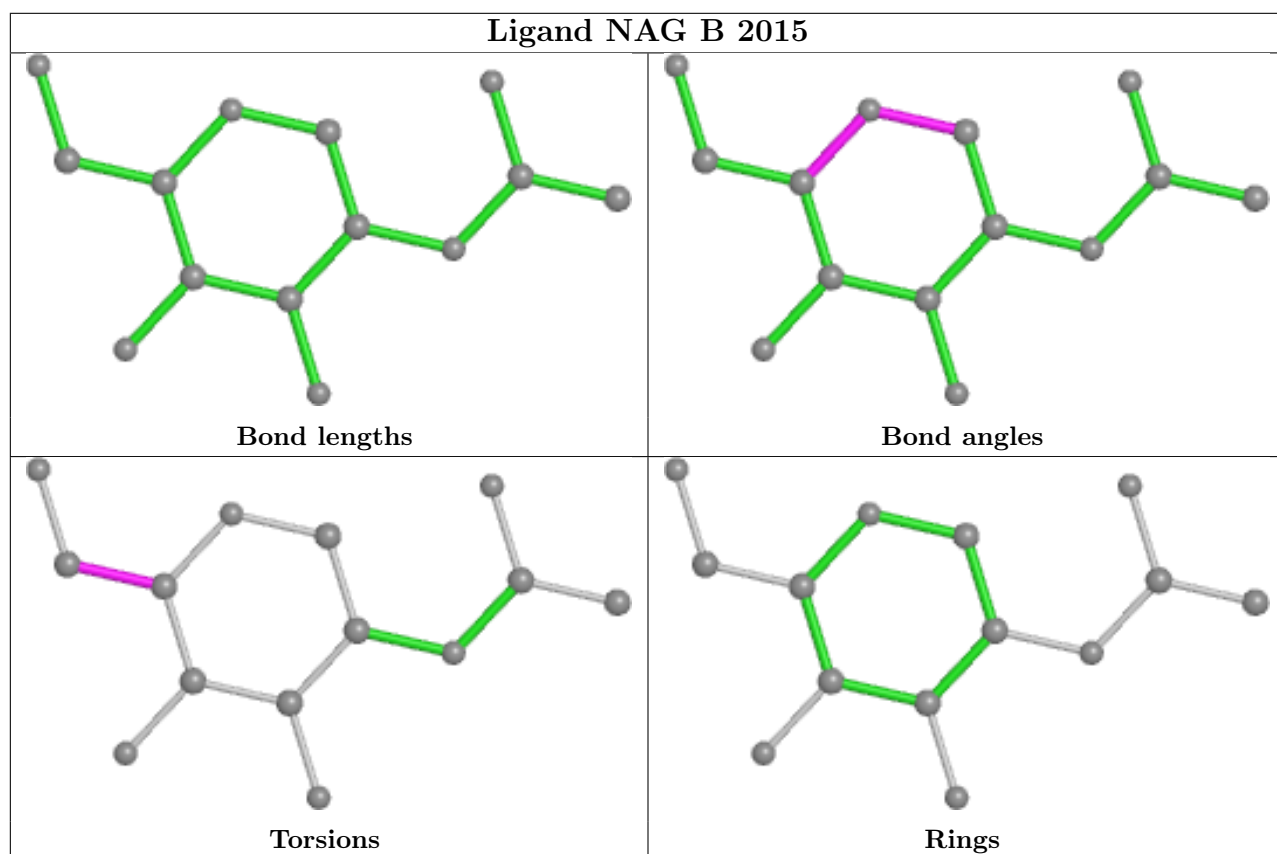
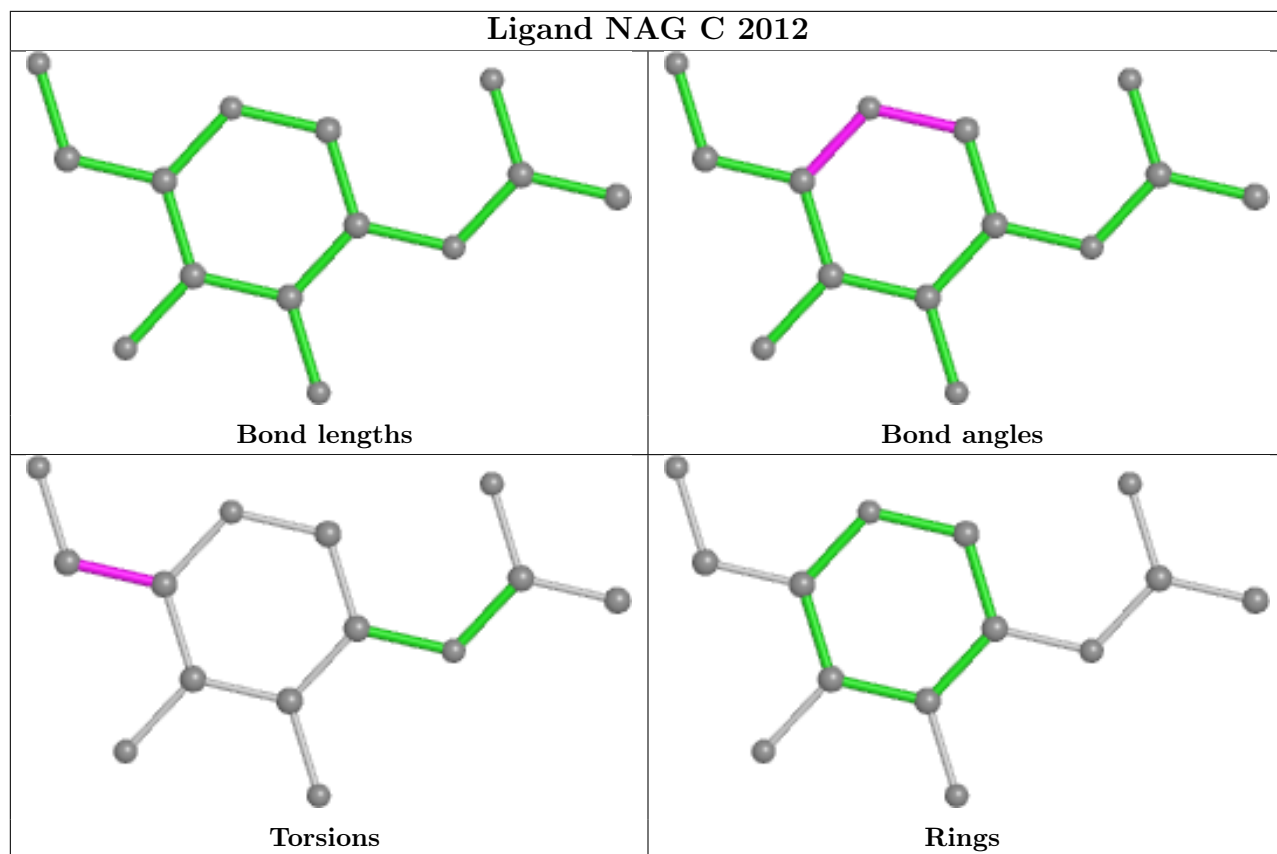
2 monomers are involved in 2 short contacts:

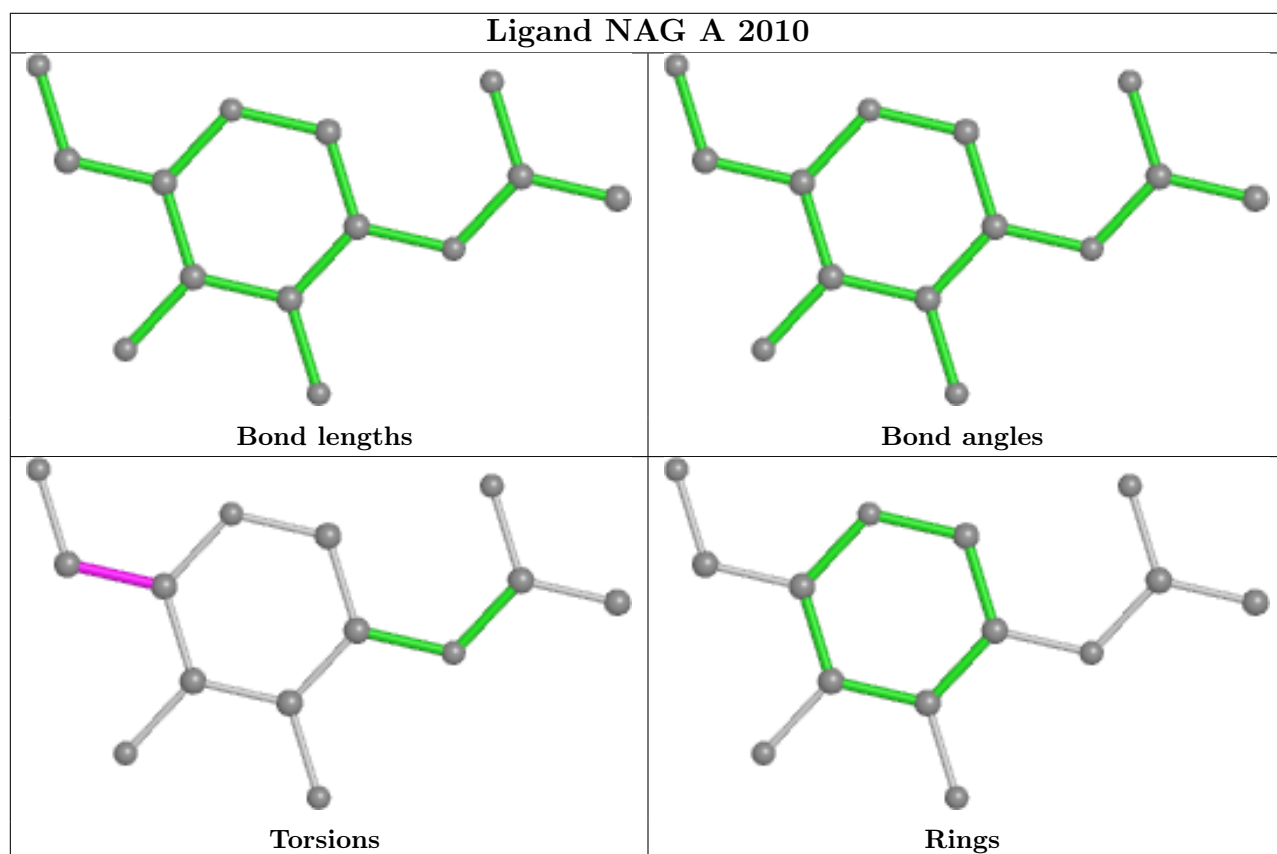
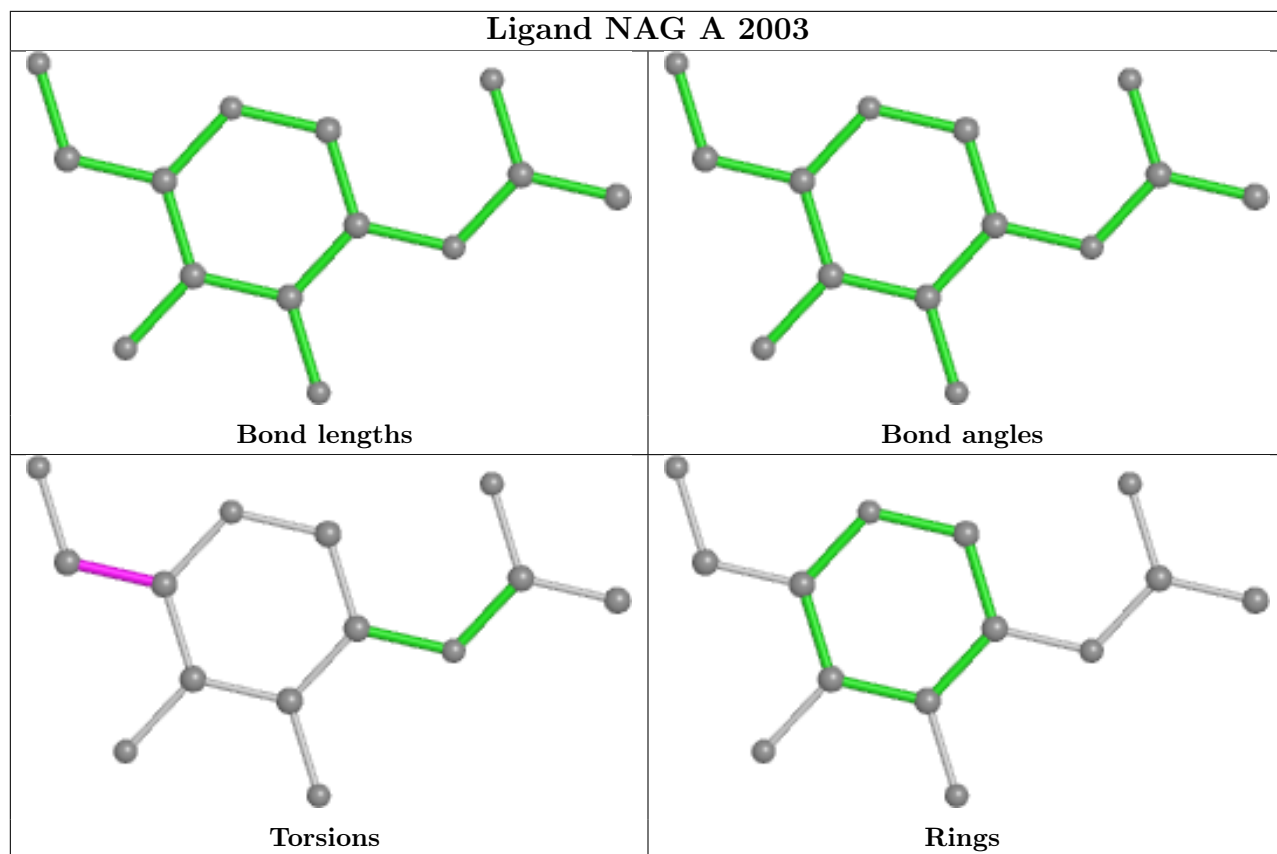
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2006	NAG	1	0
4	A	2016	NAG	1	0

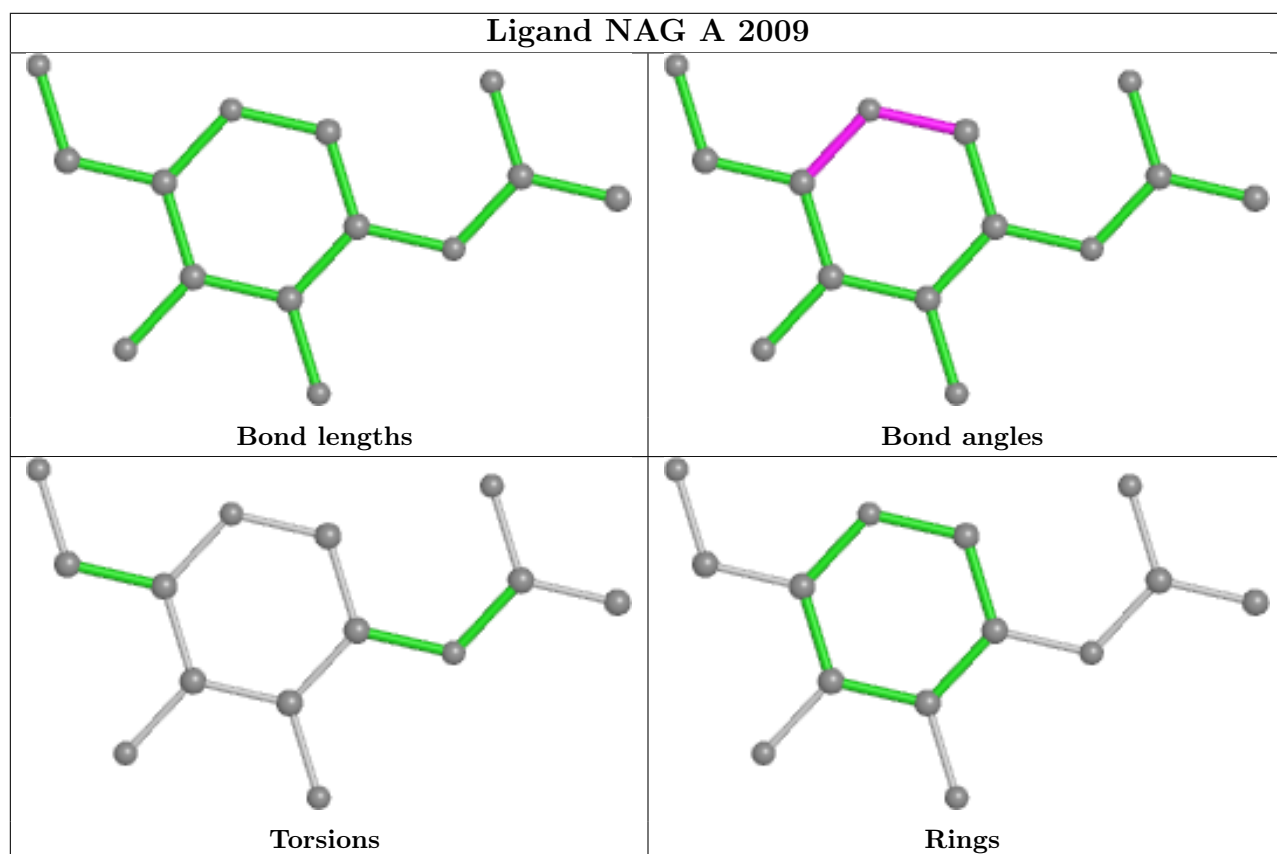
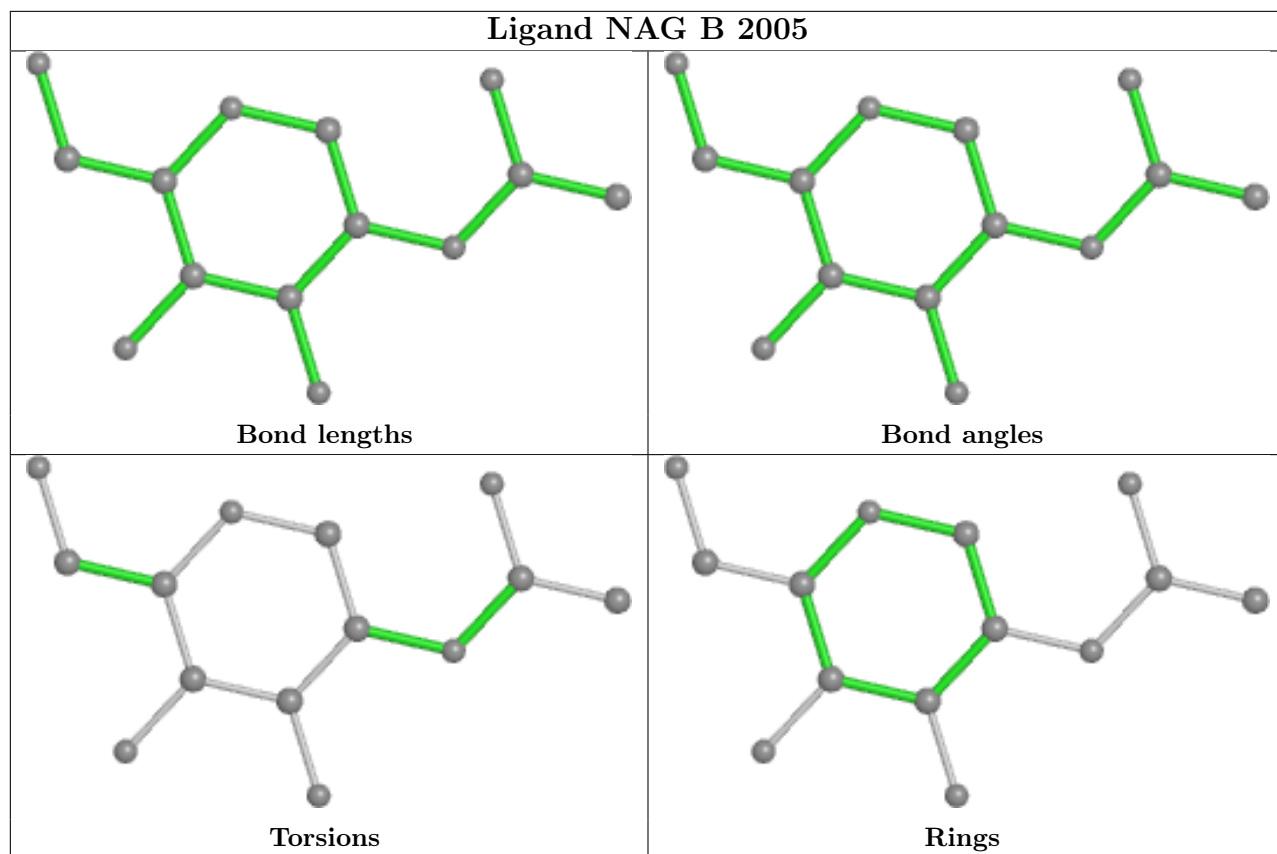
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

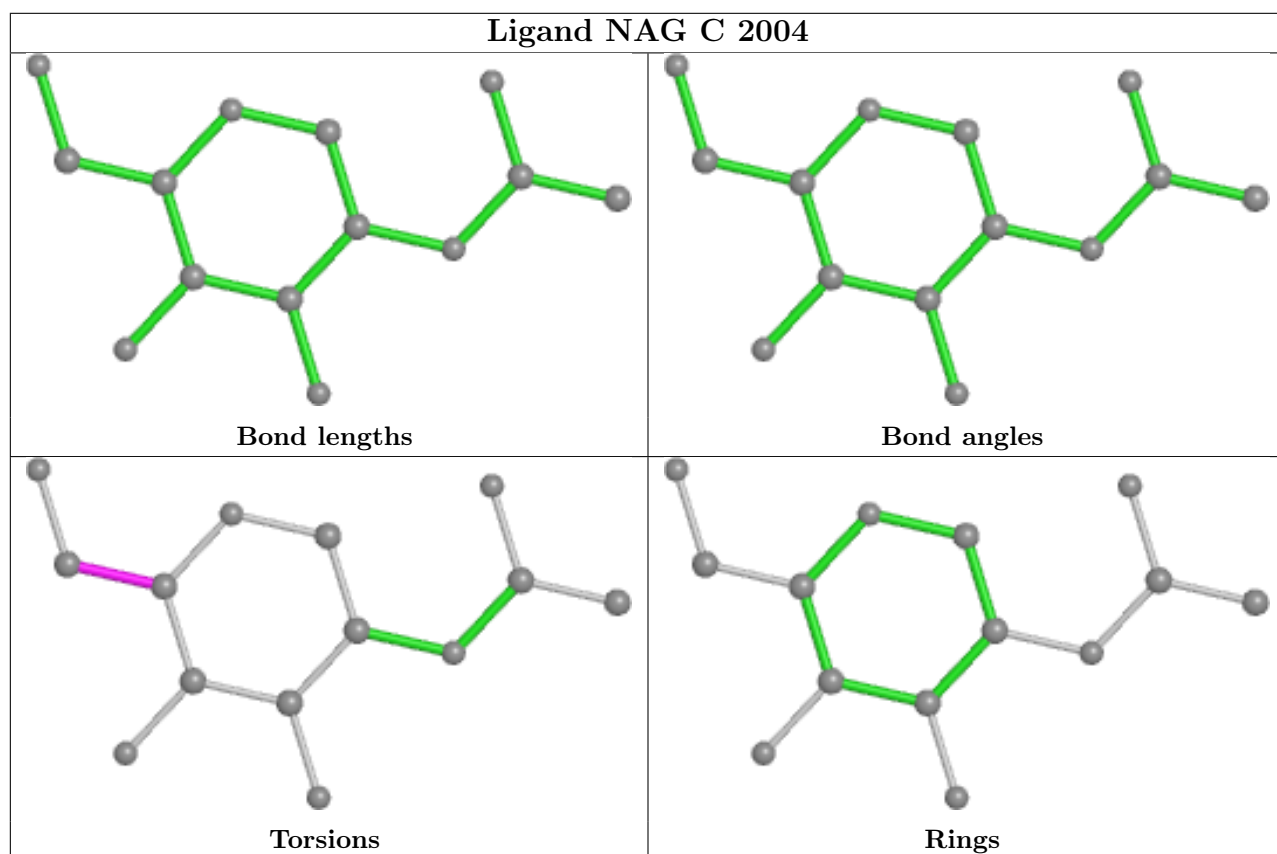
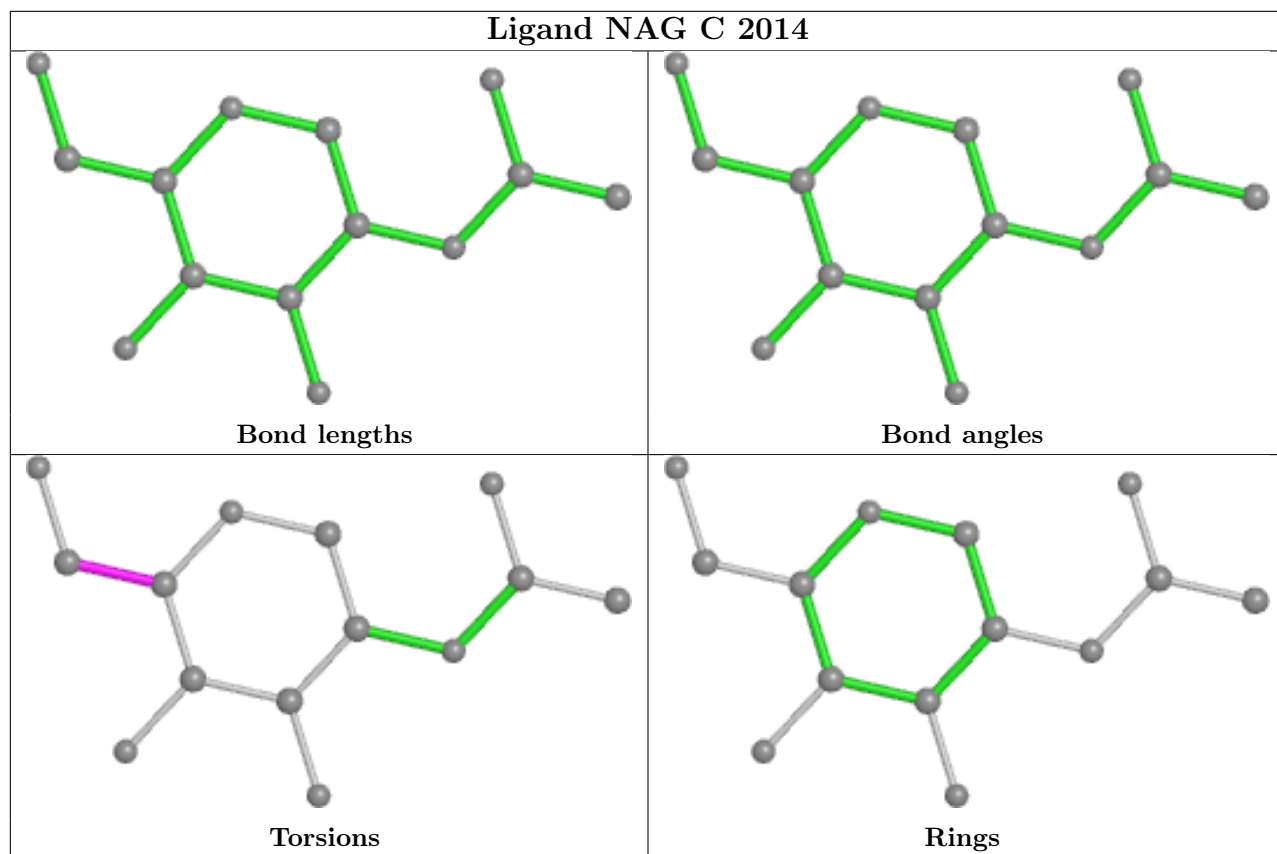




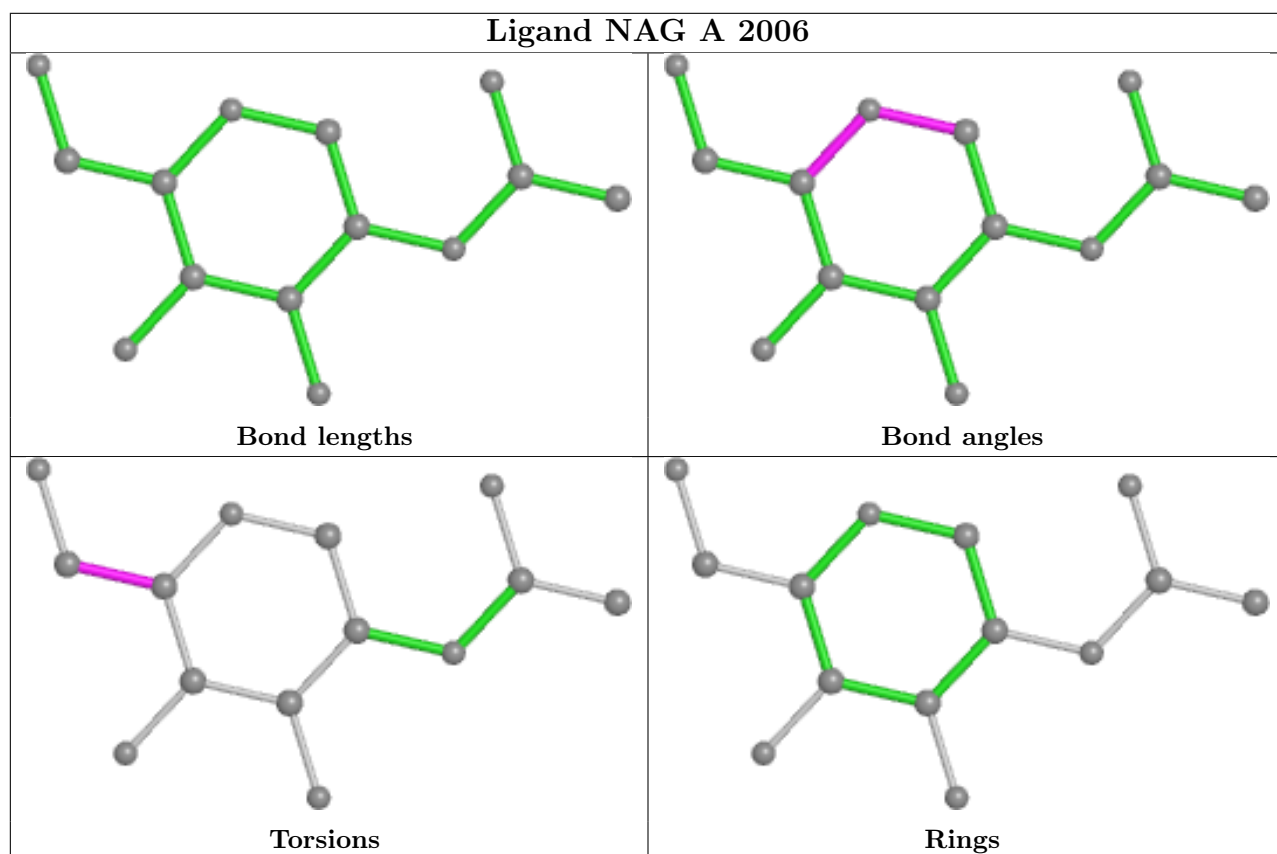
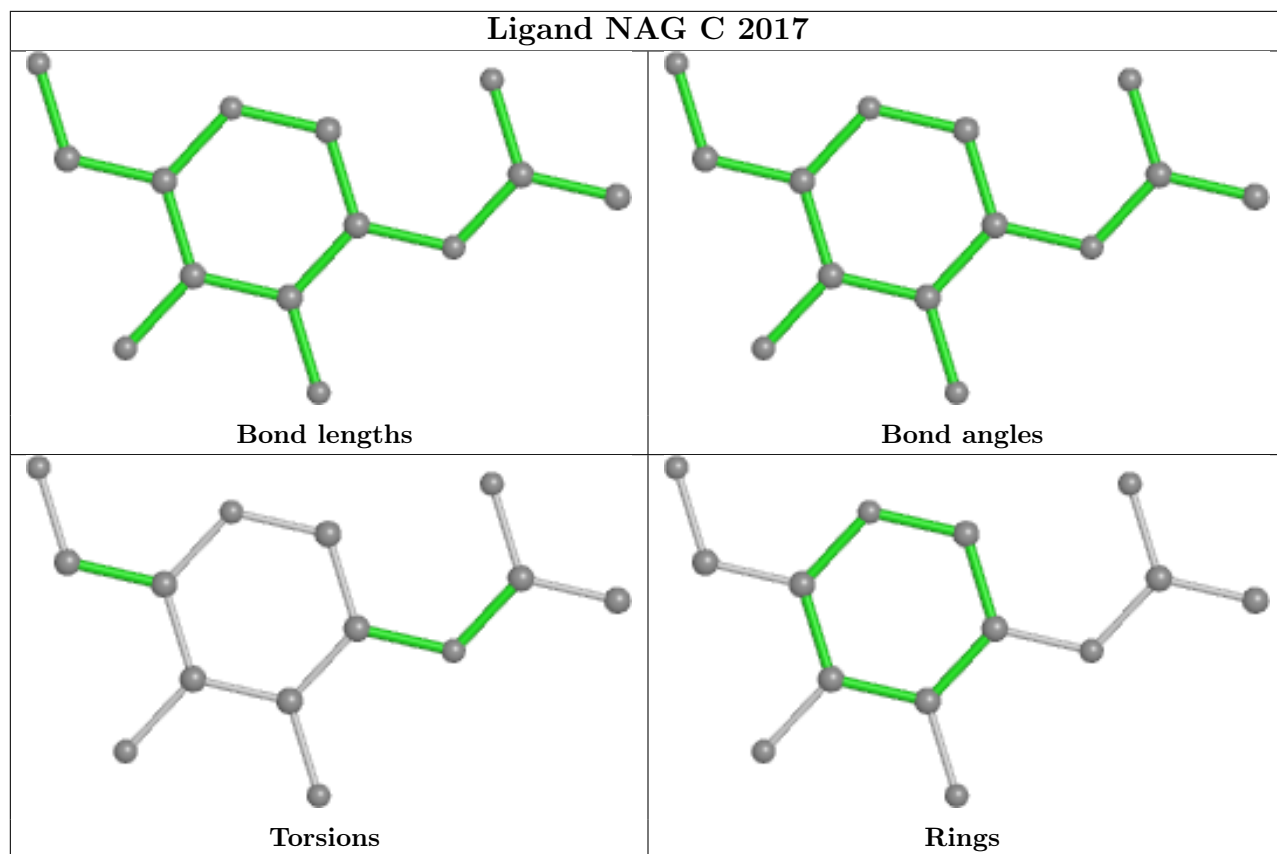


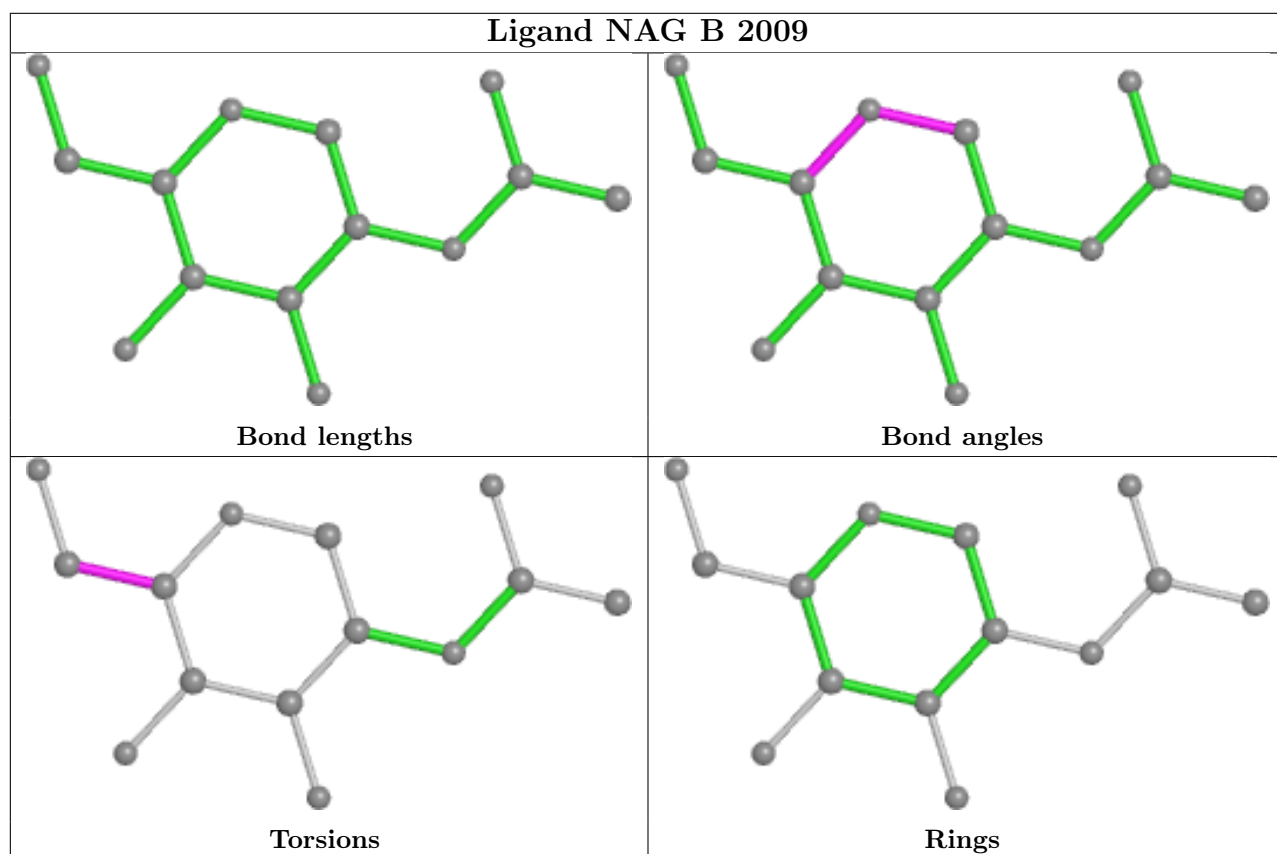
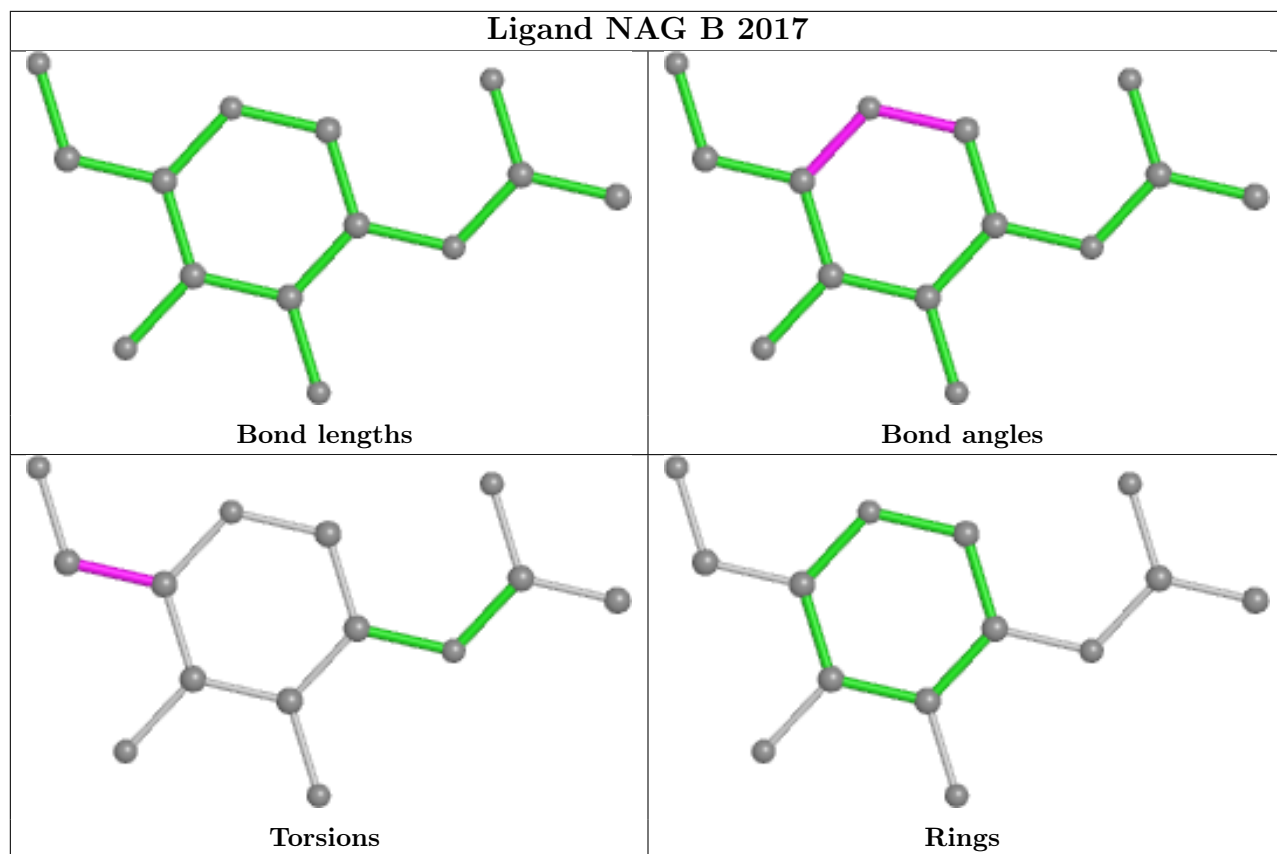


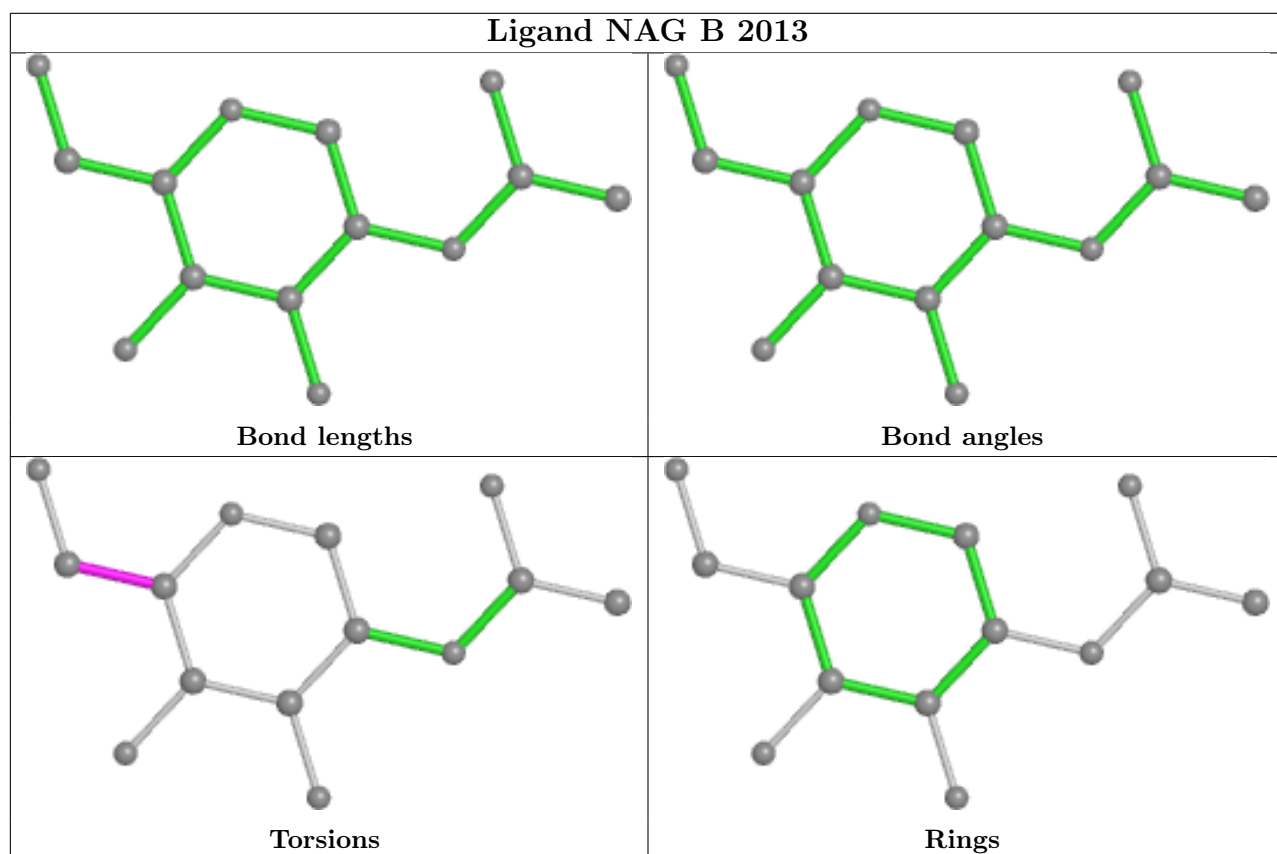
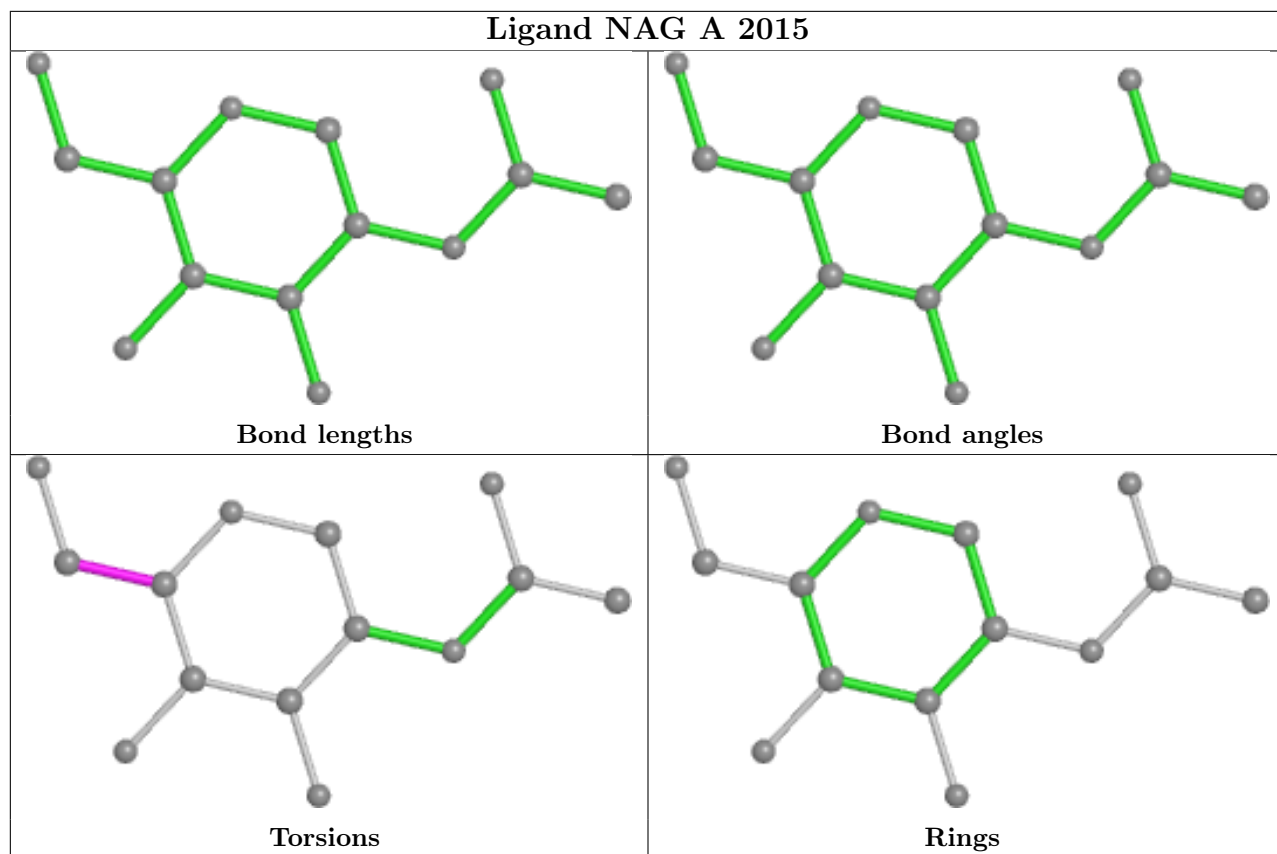


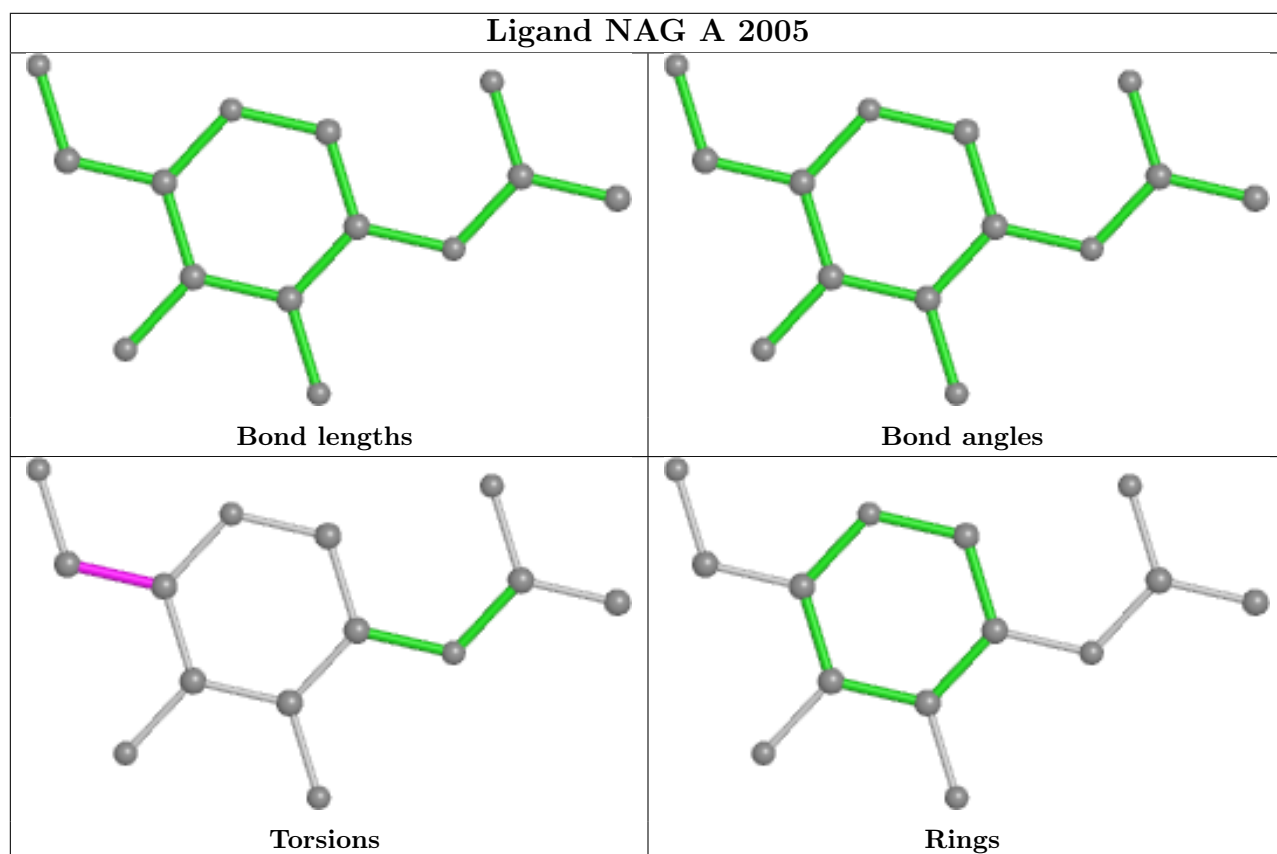
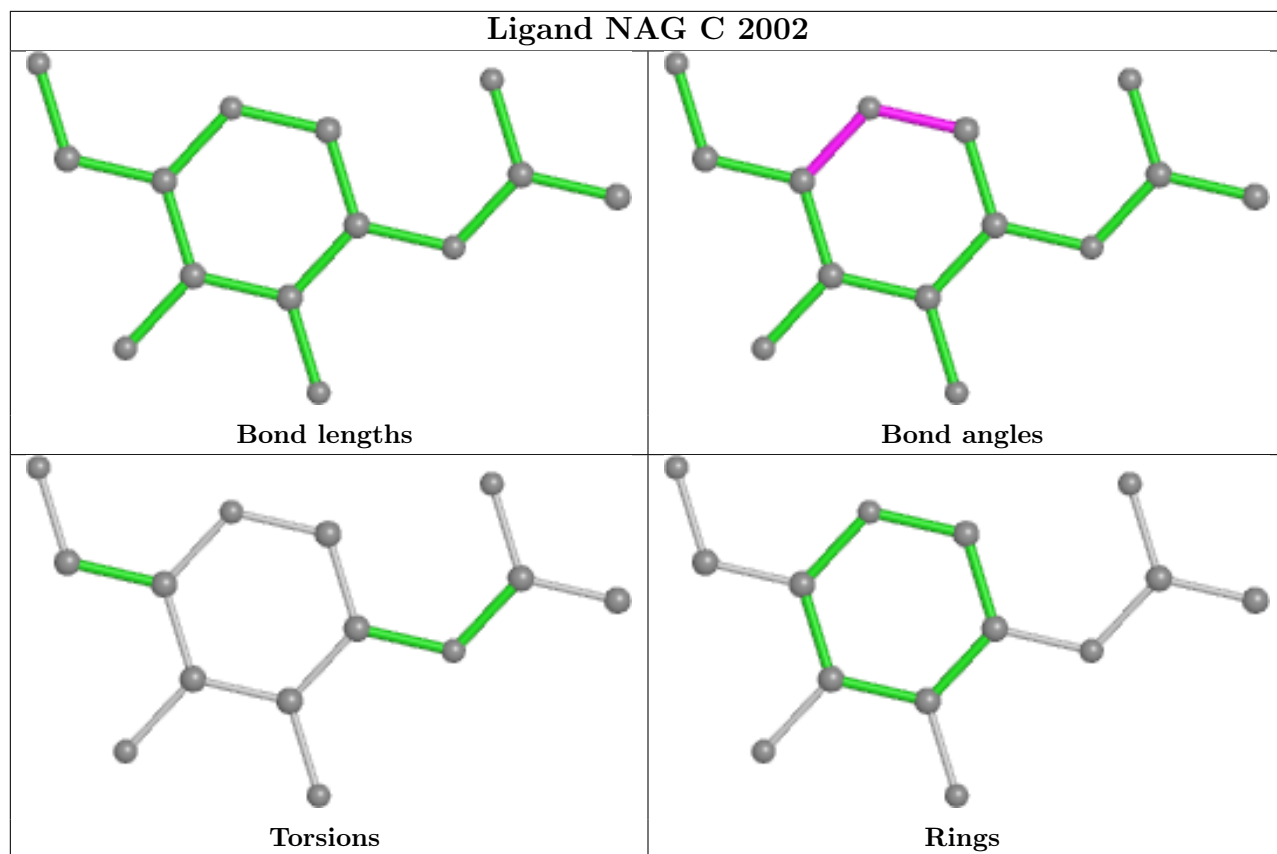


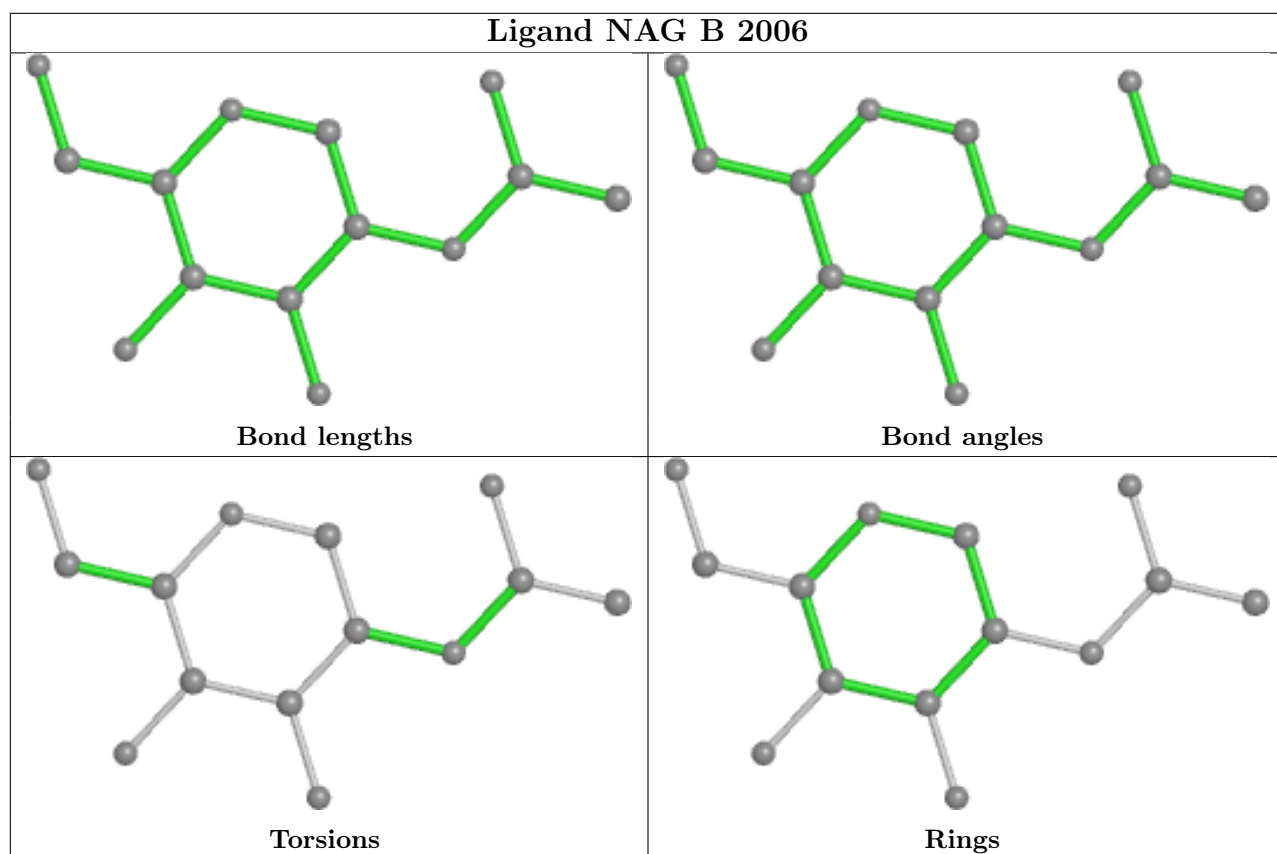
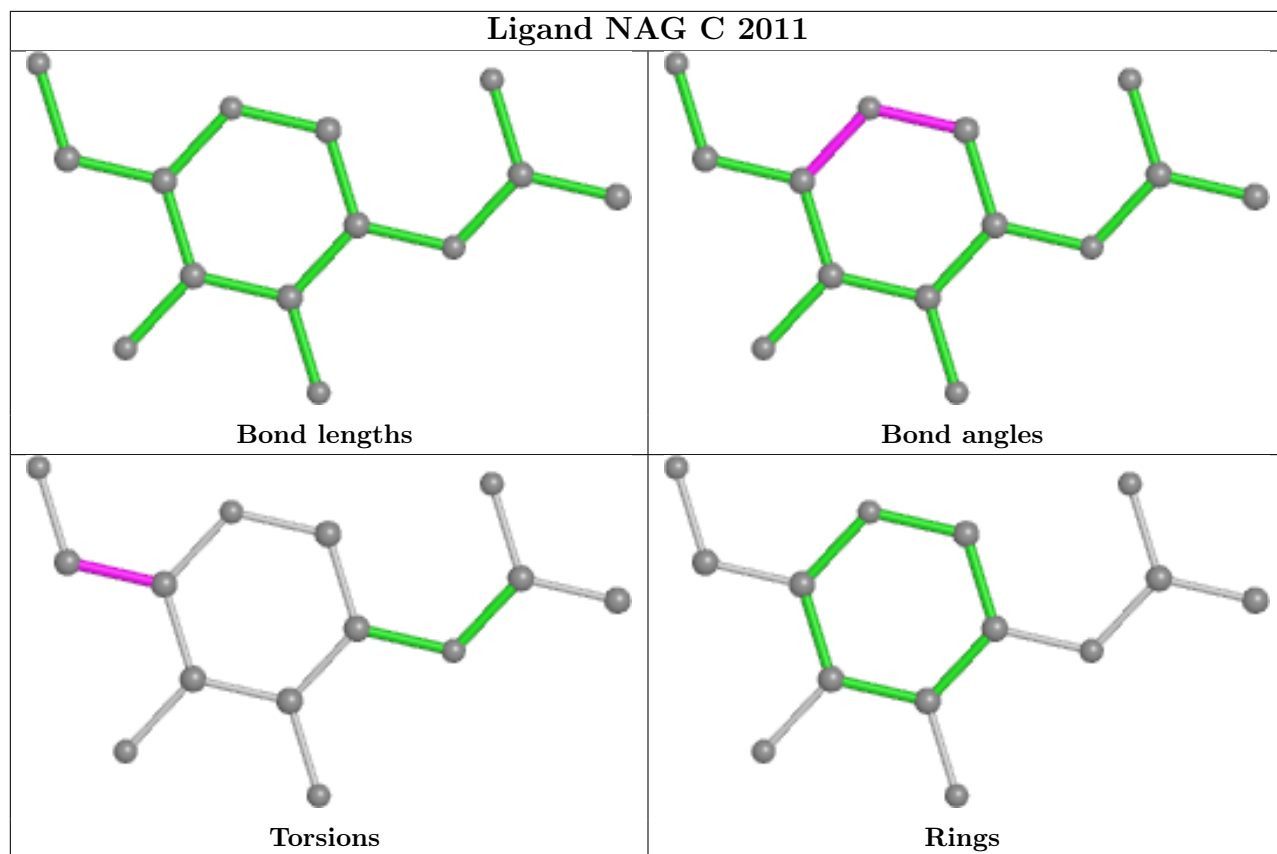


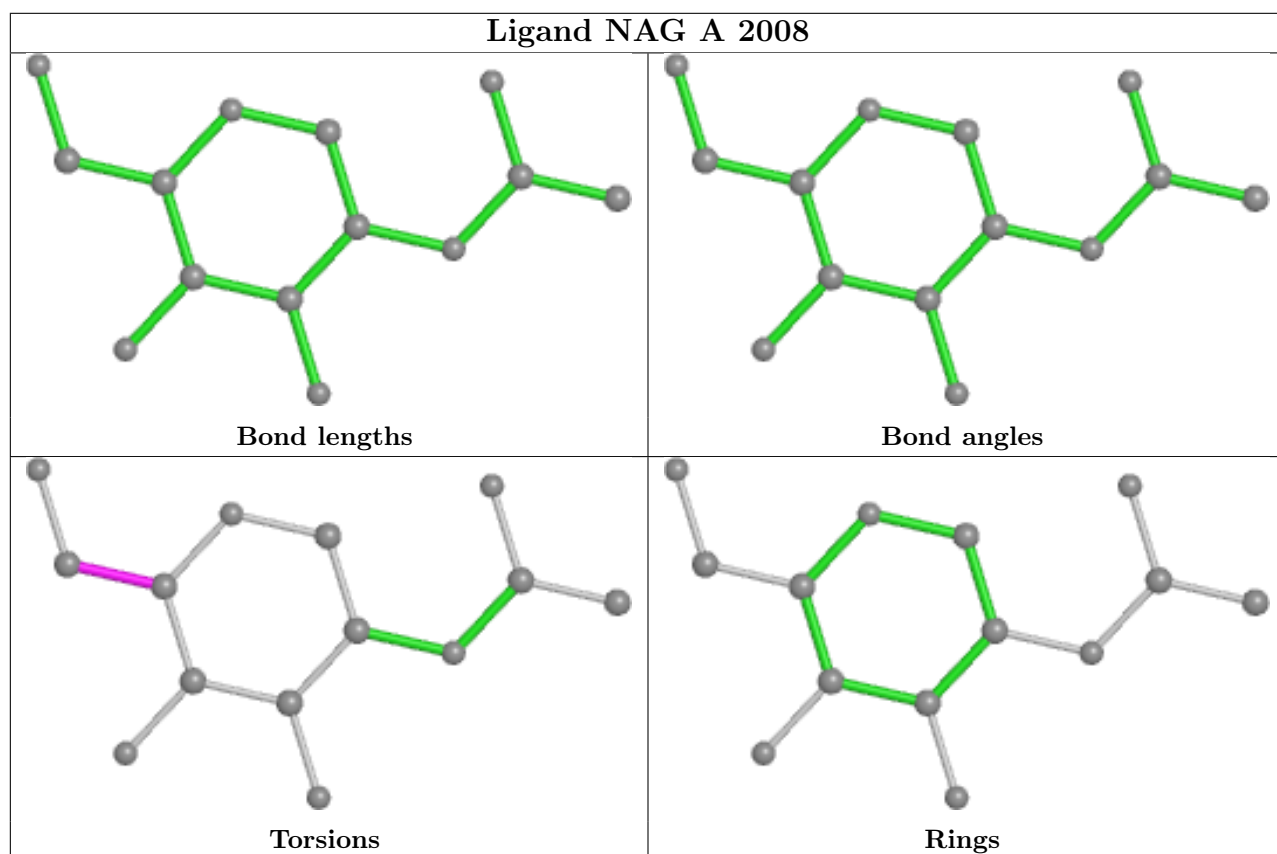
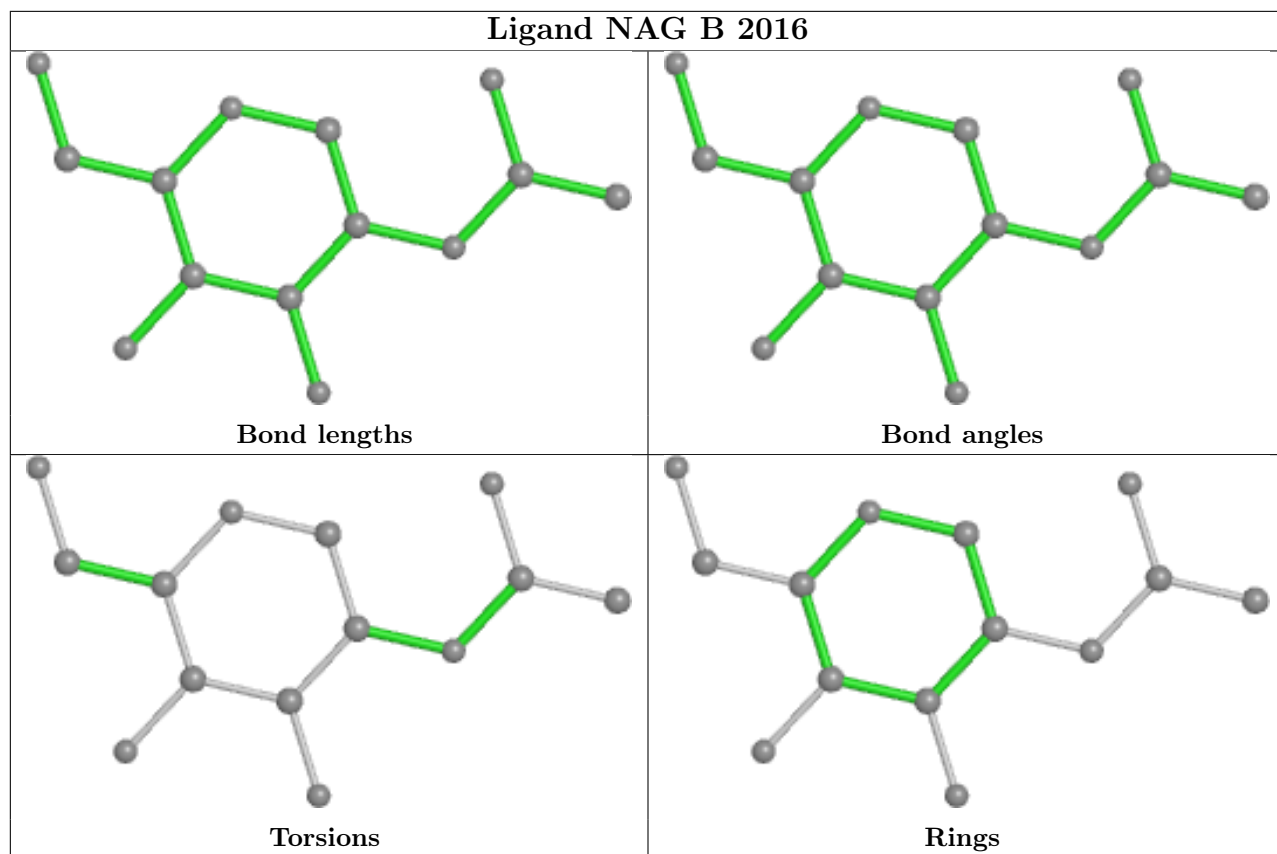


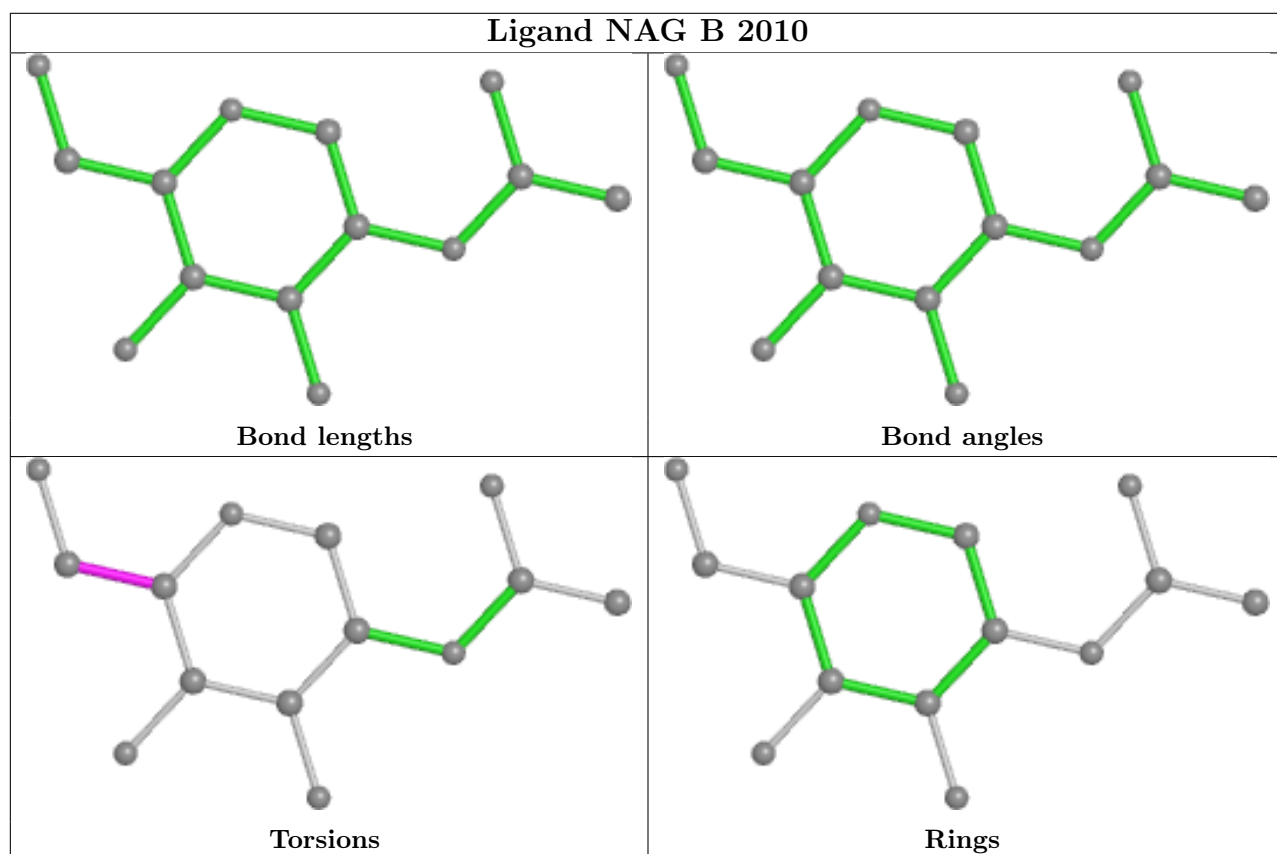
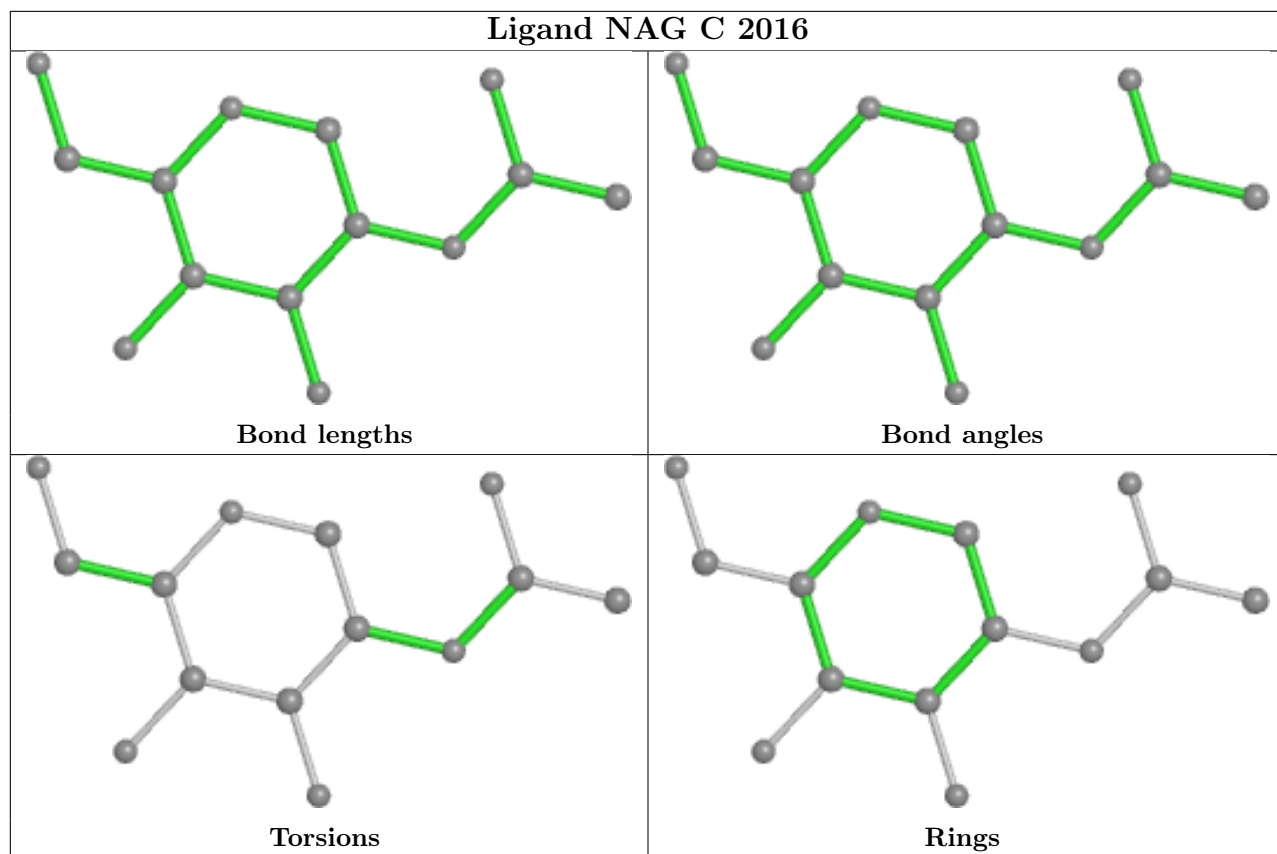


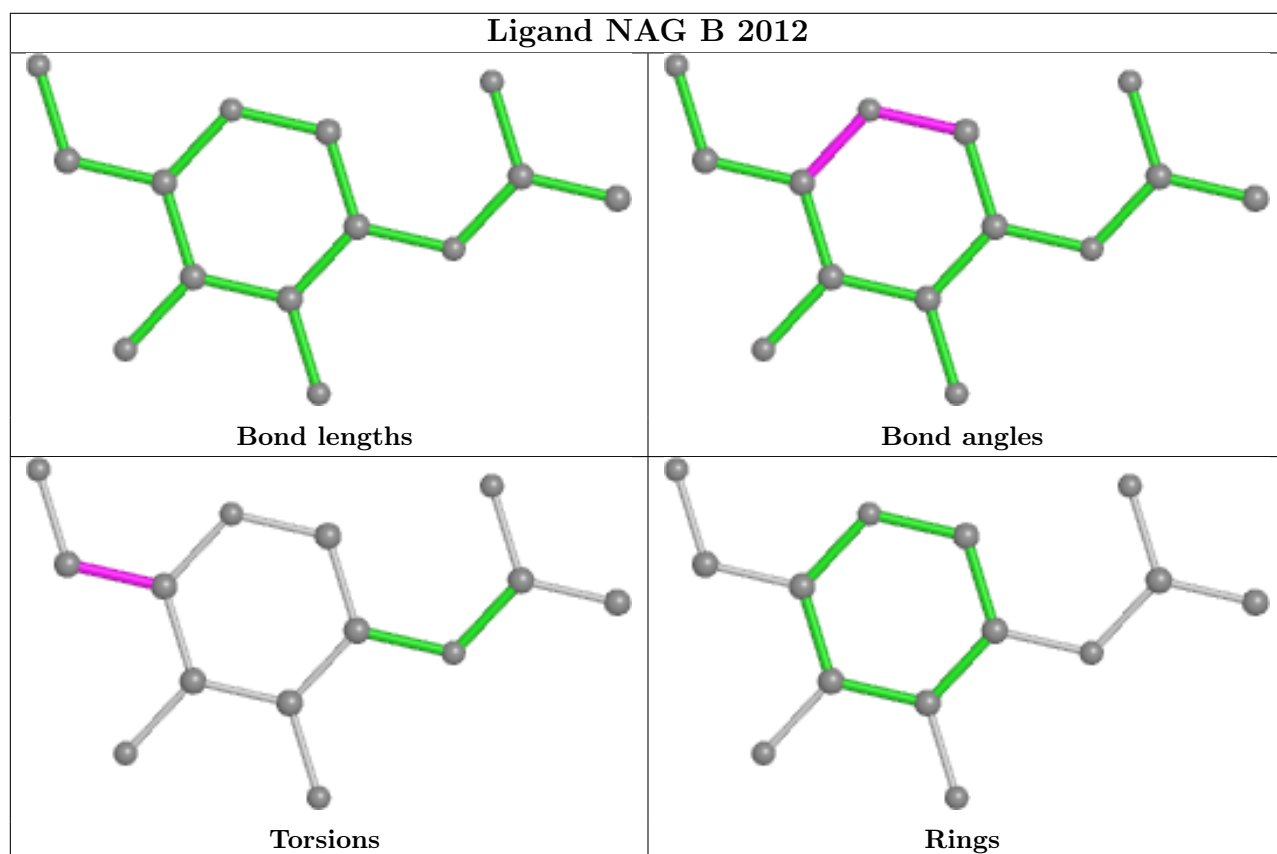
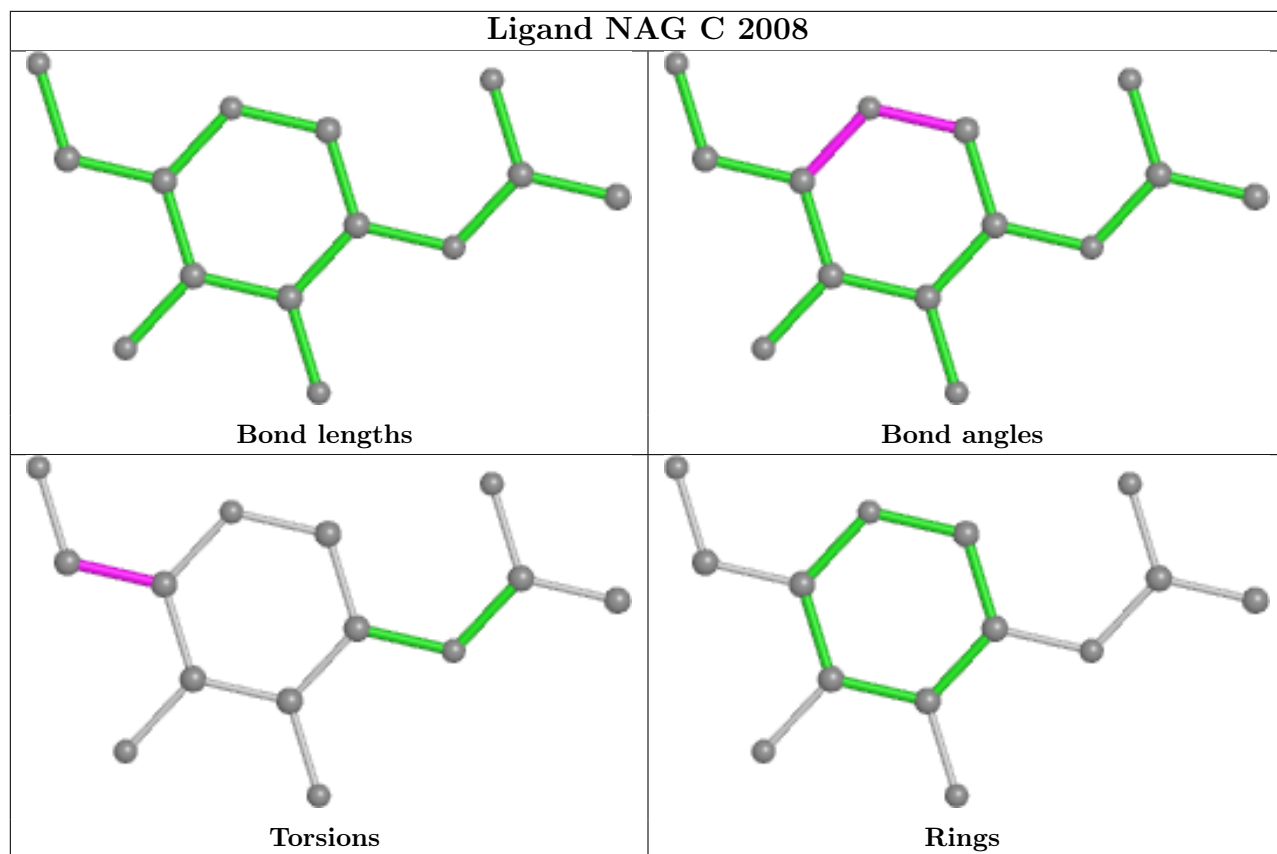




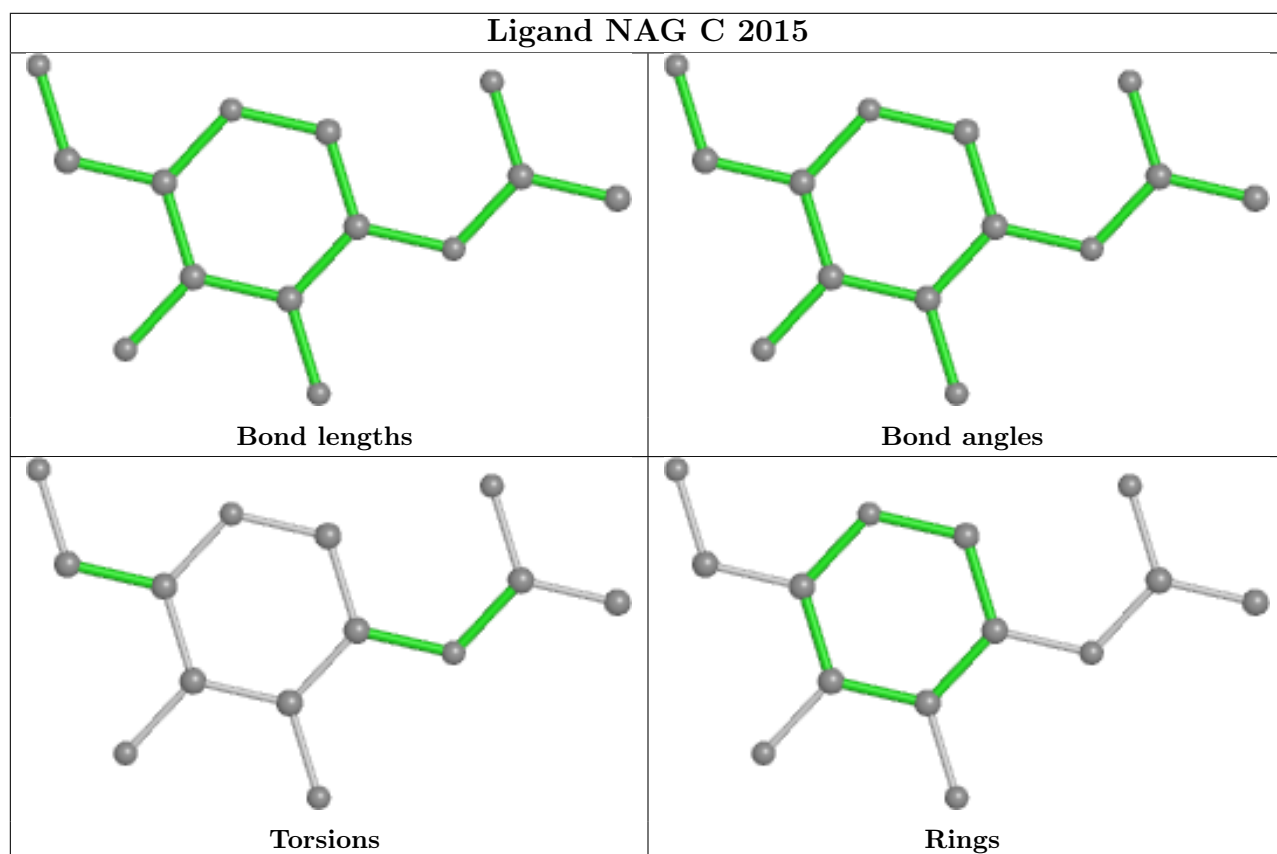
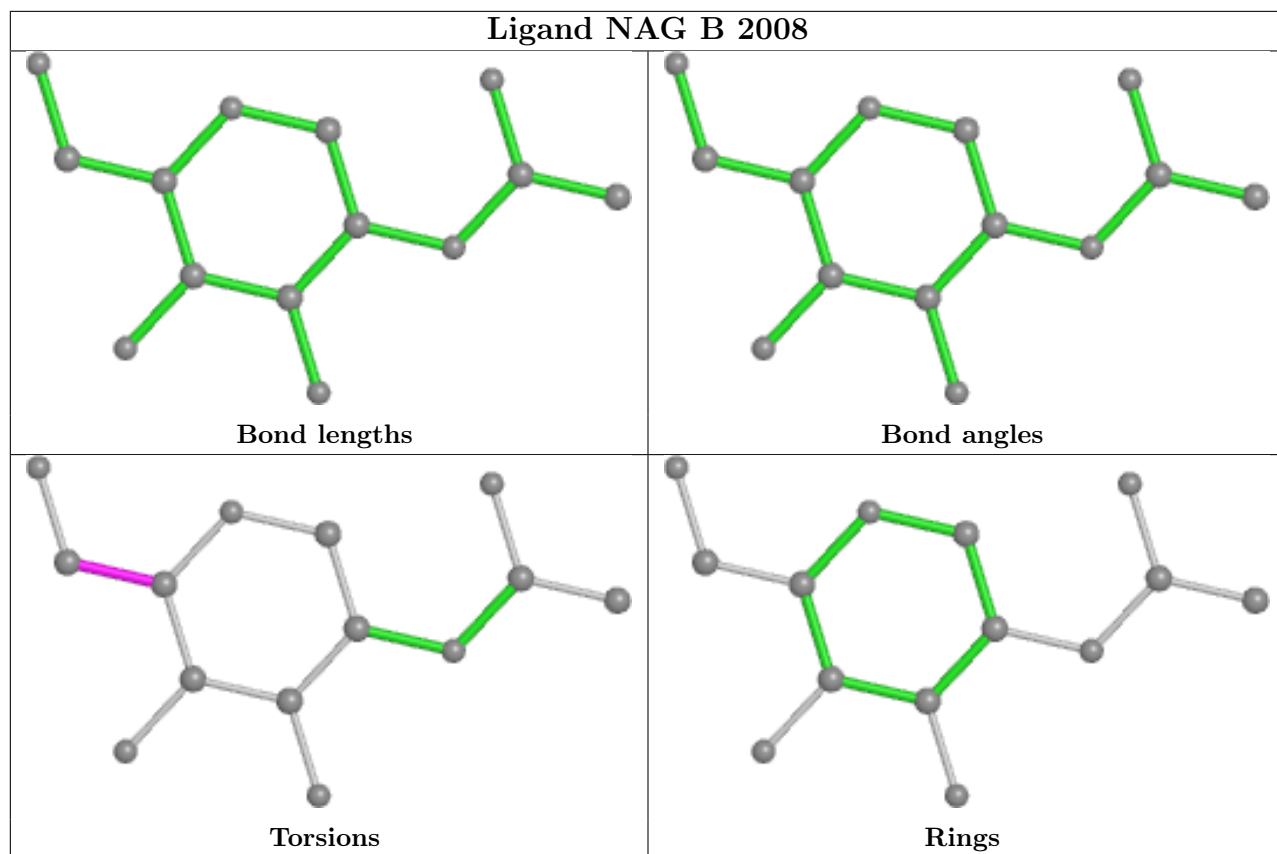


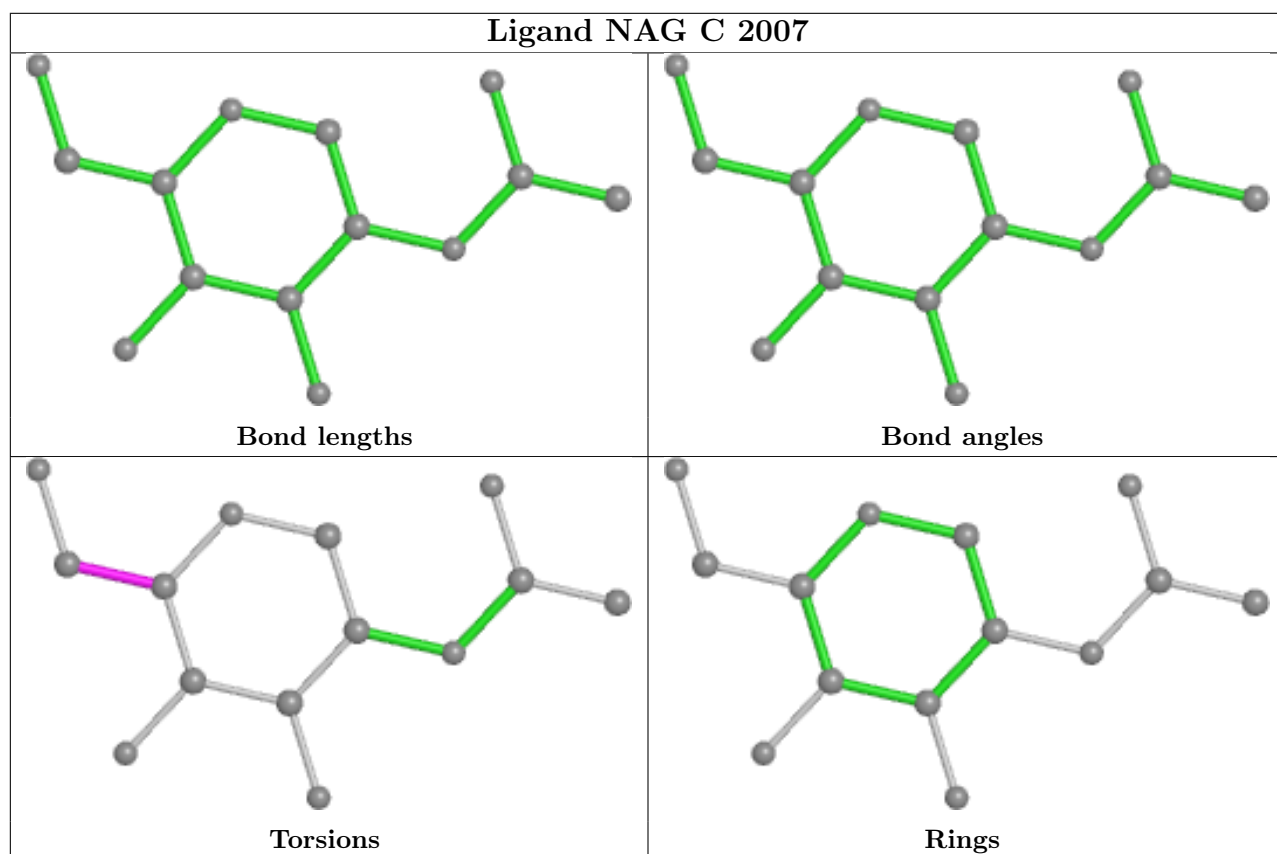
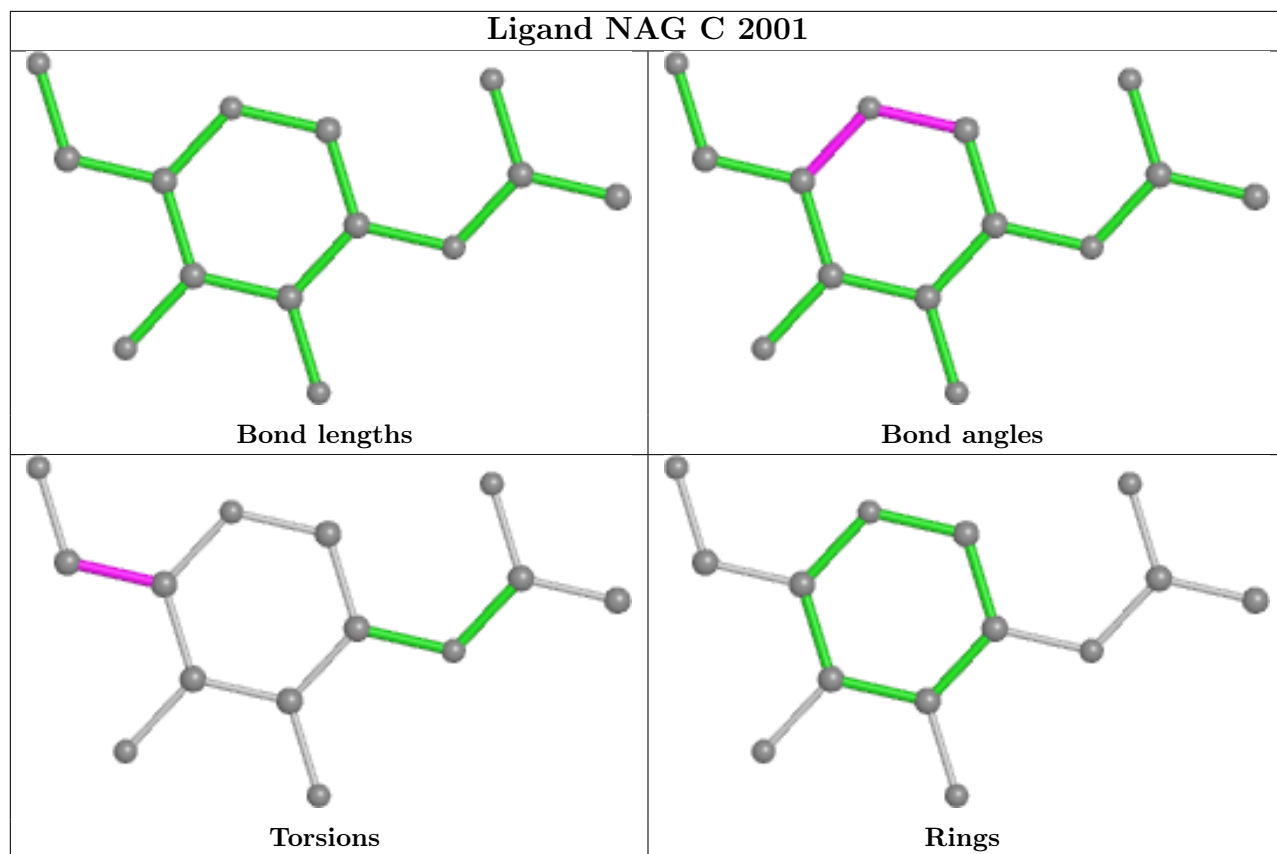


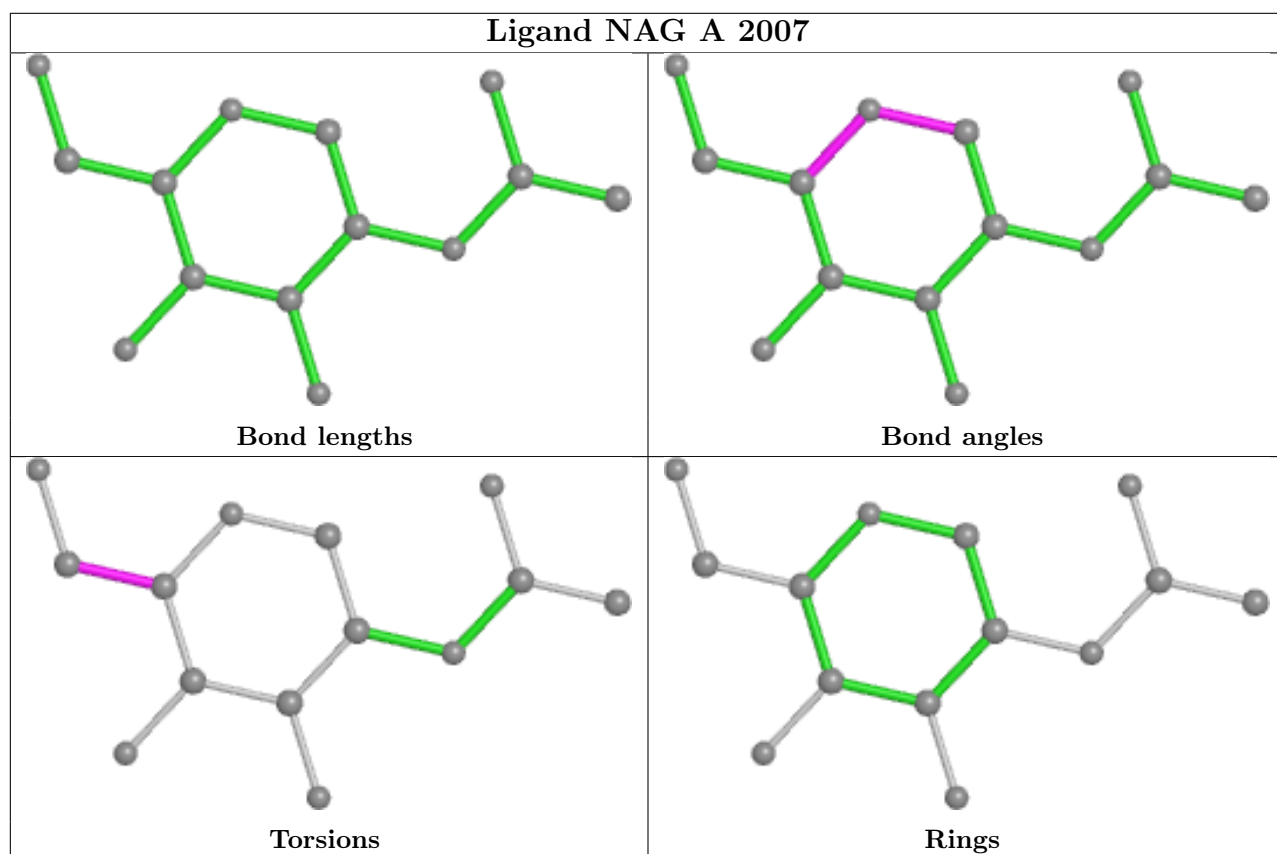
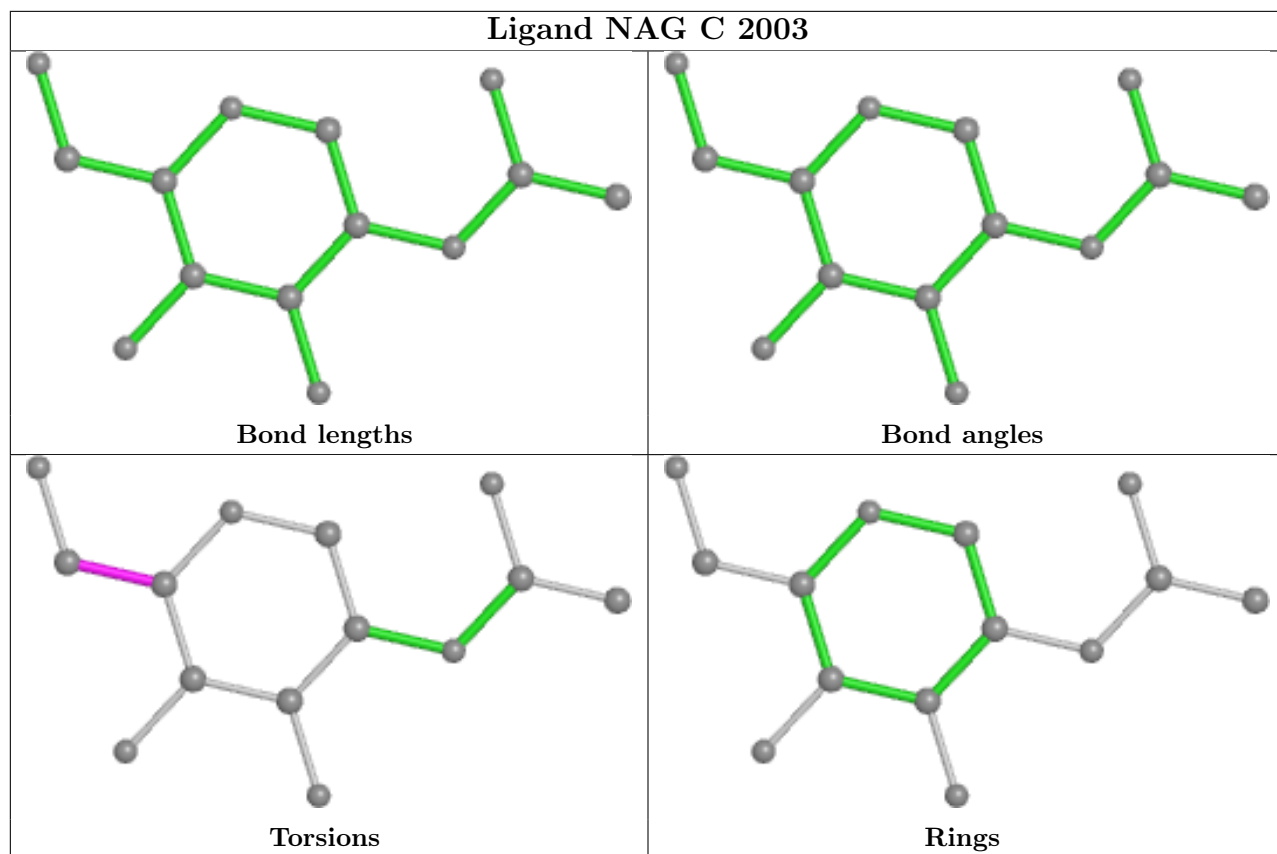


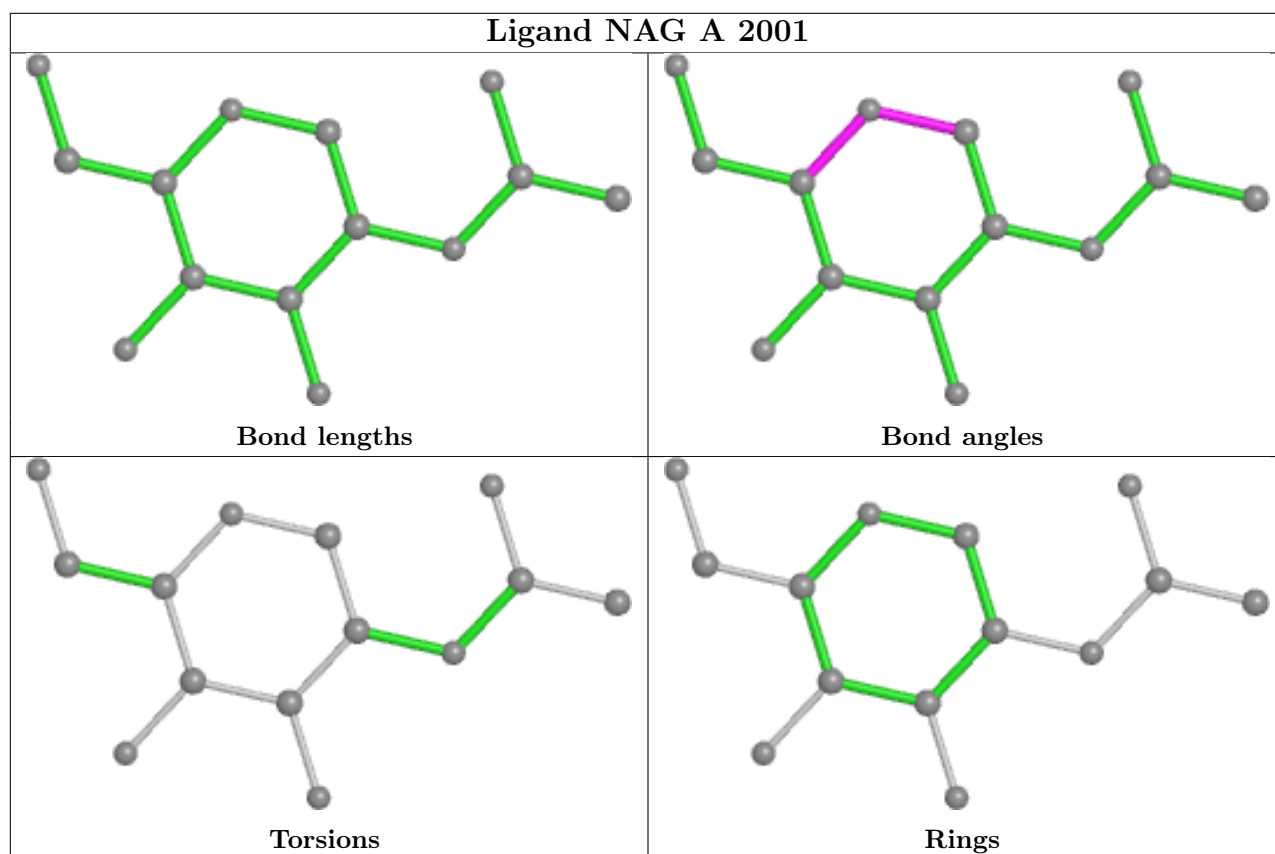
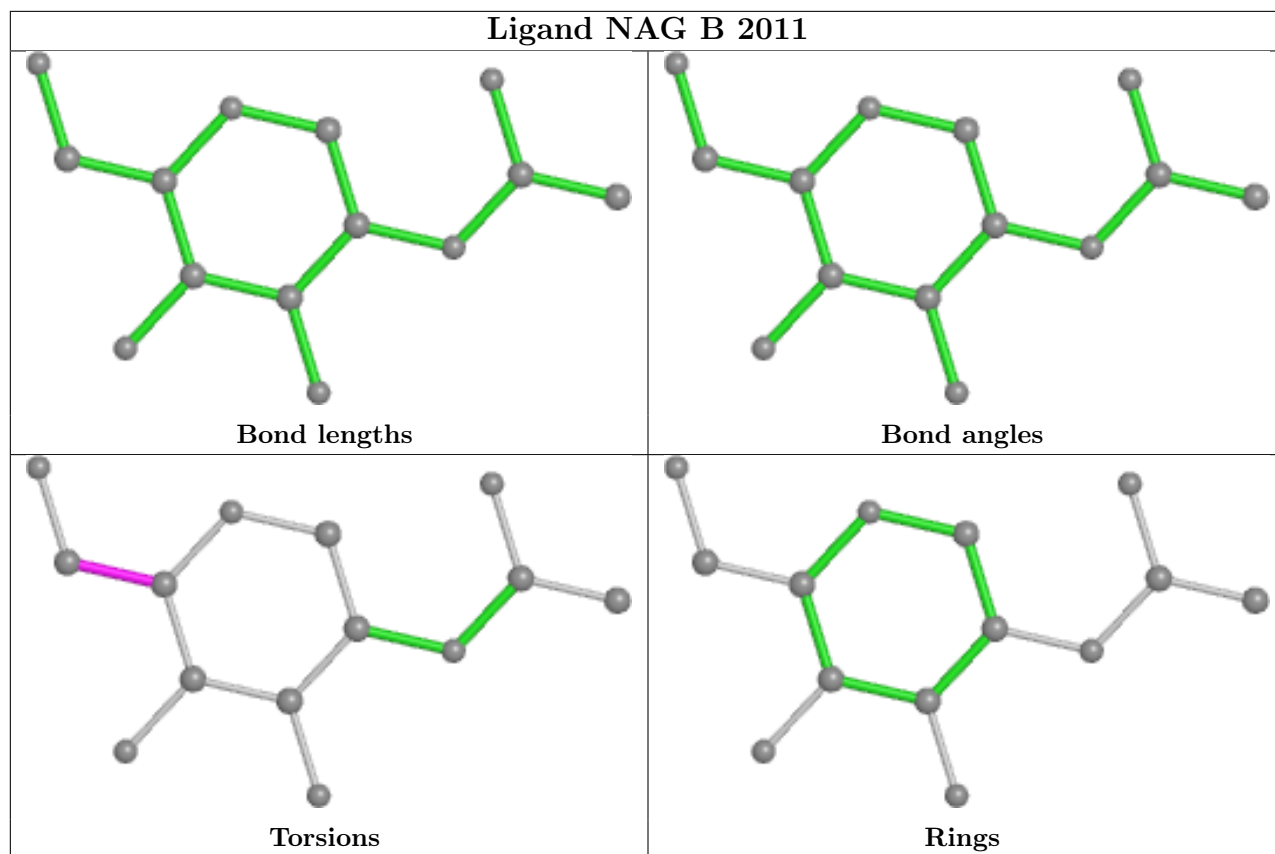


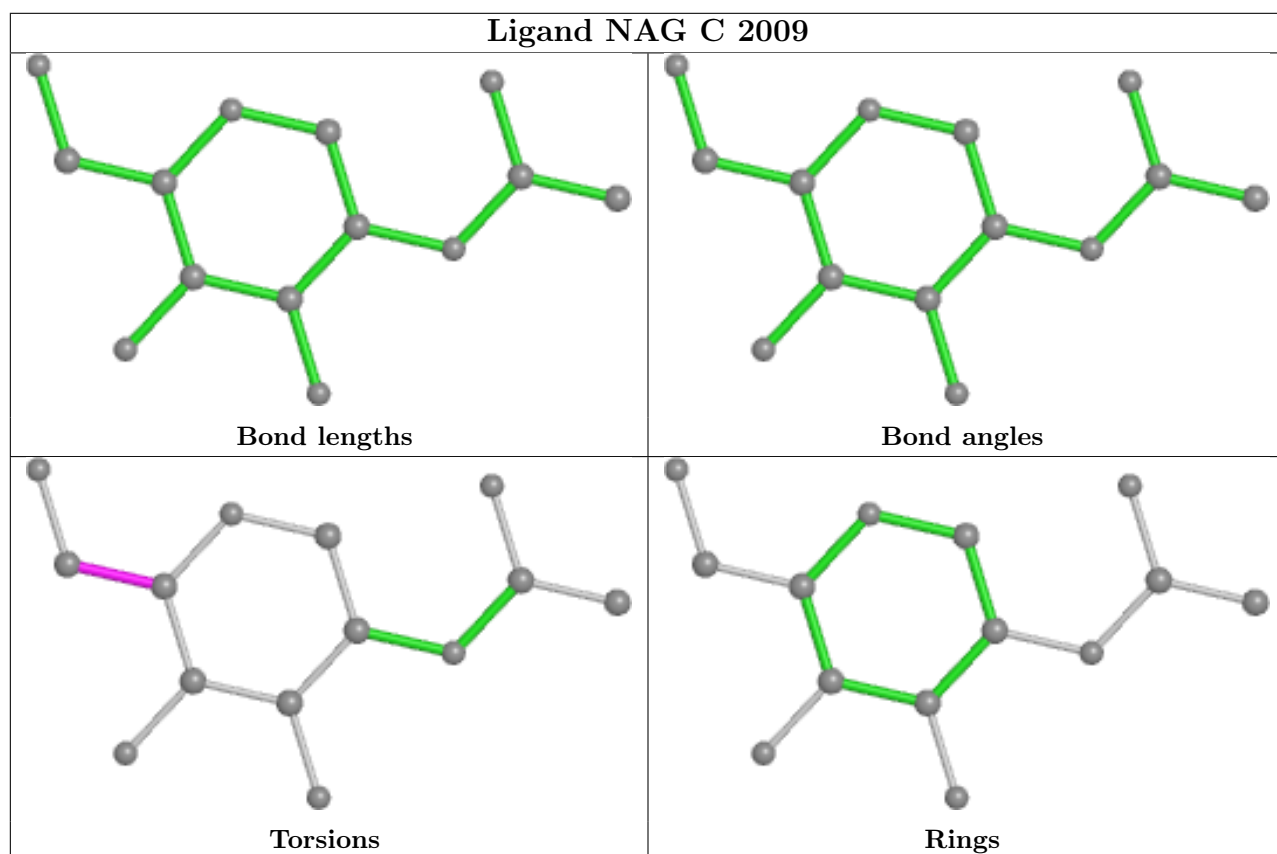
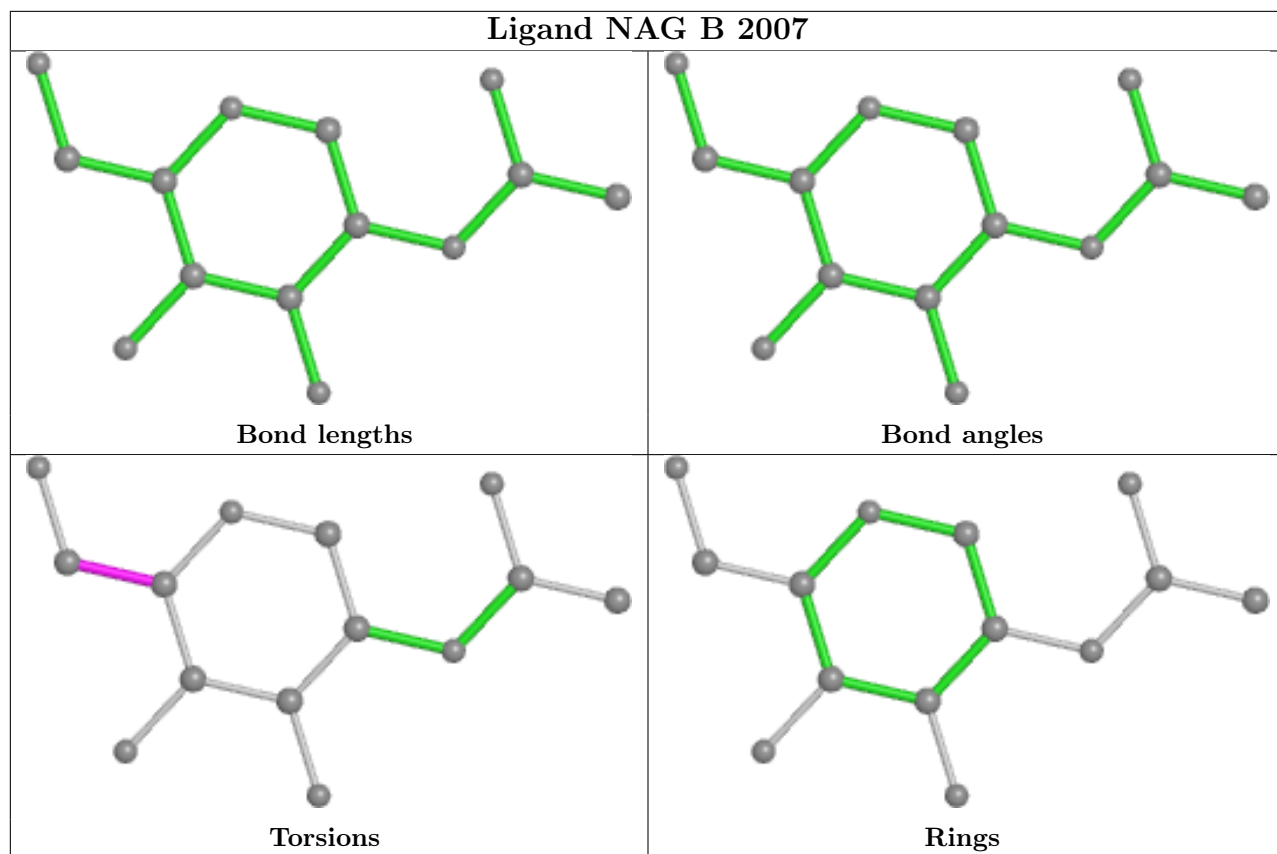


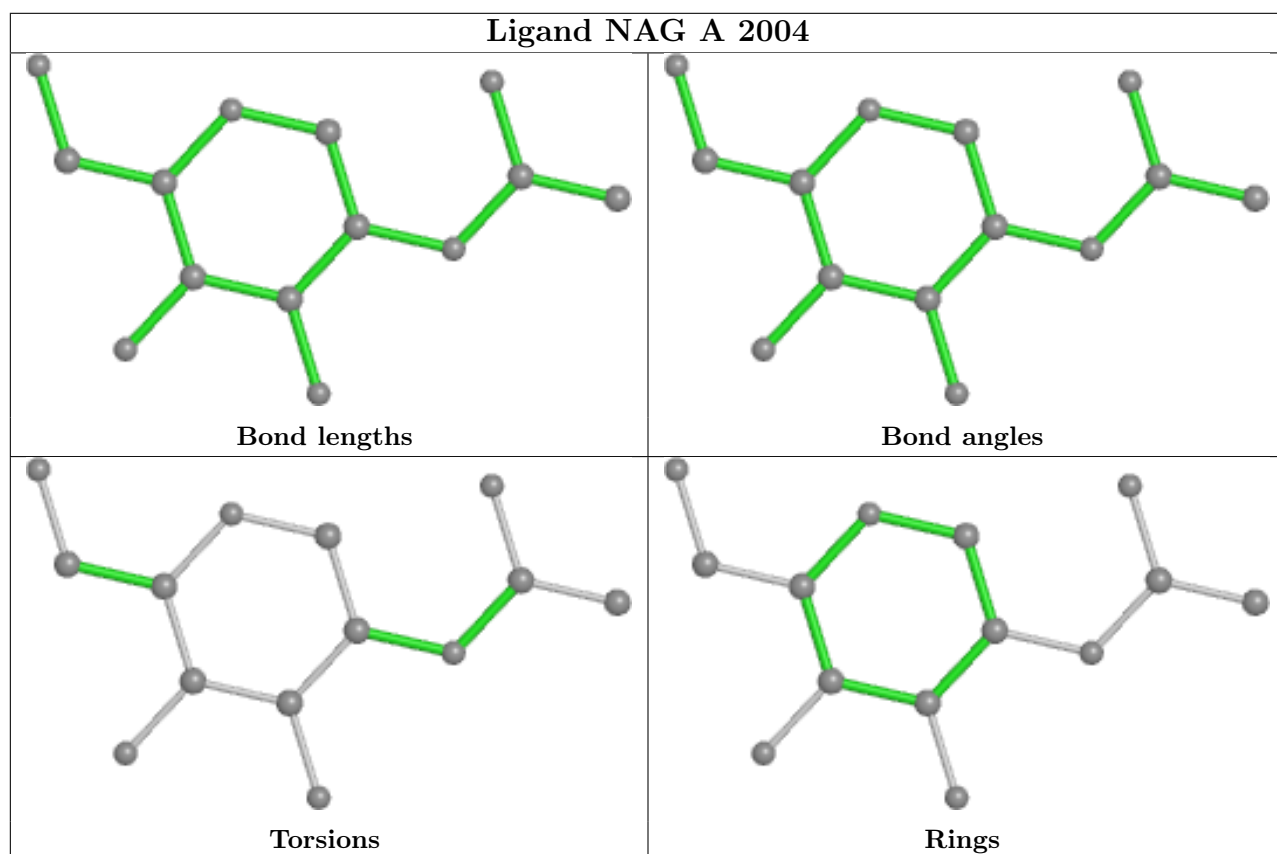
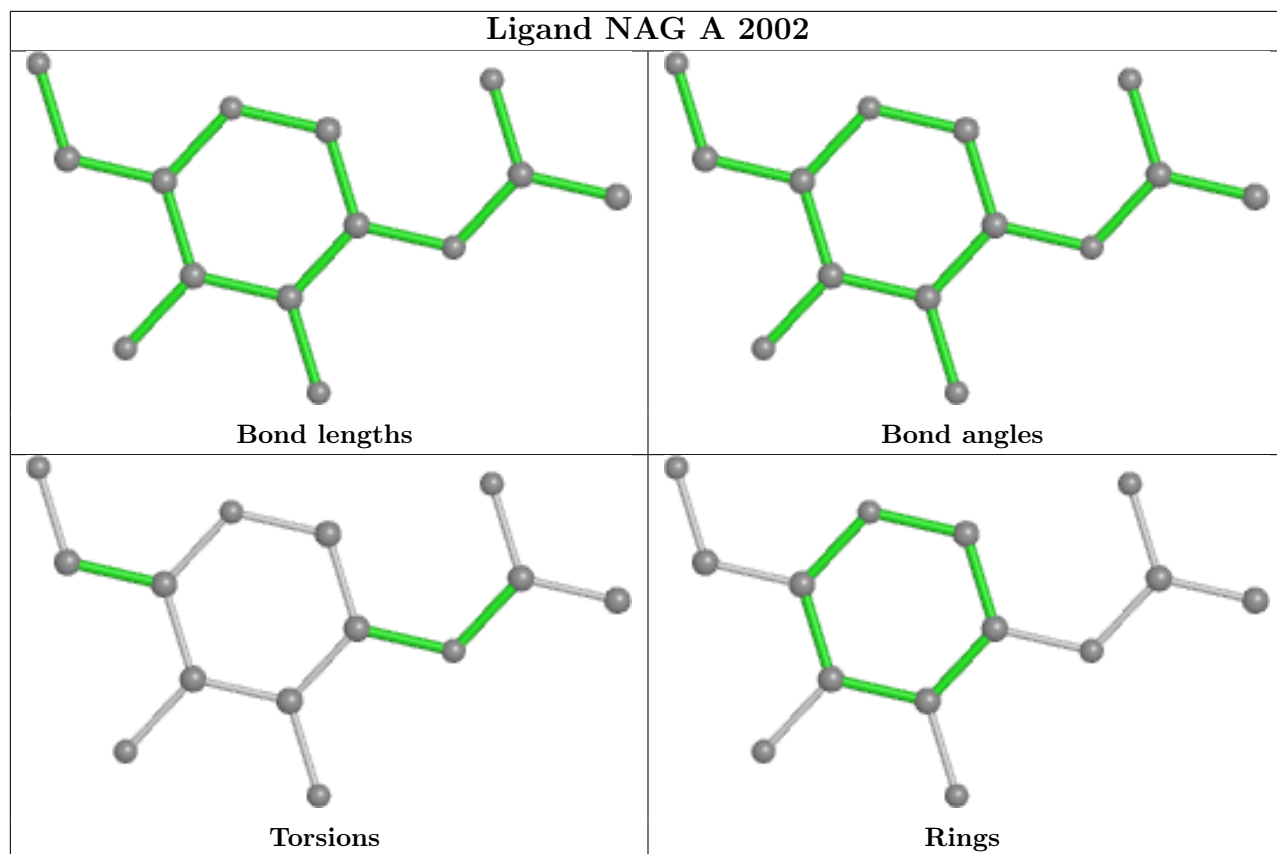


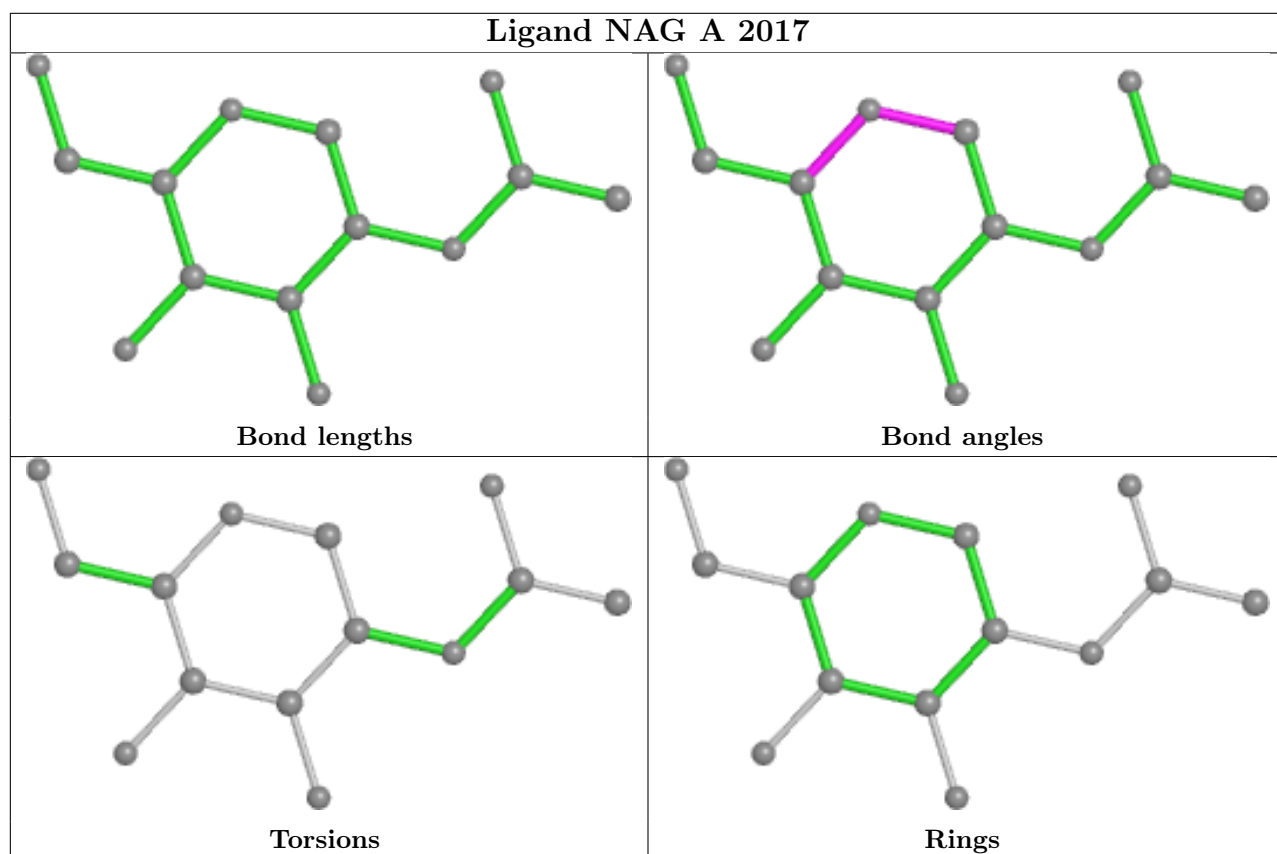
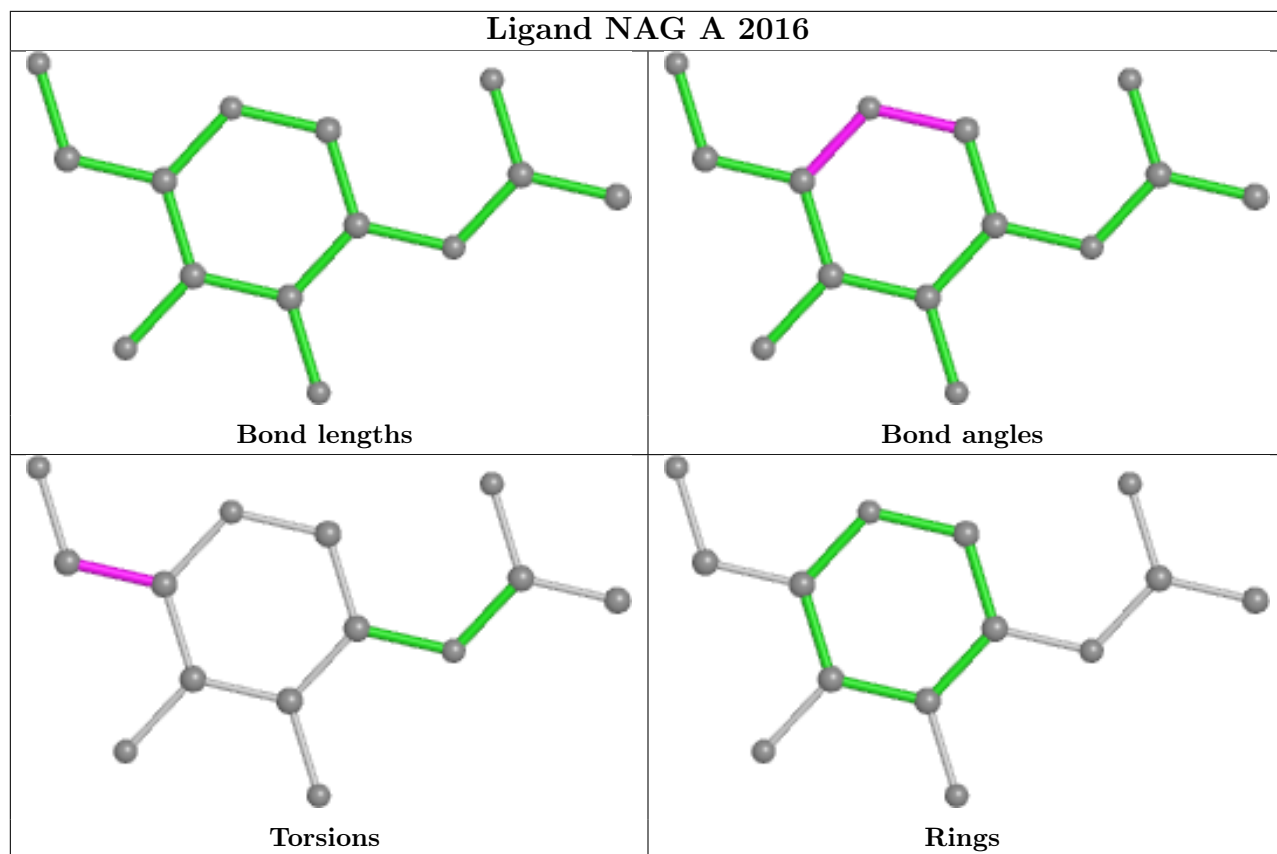


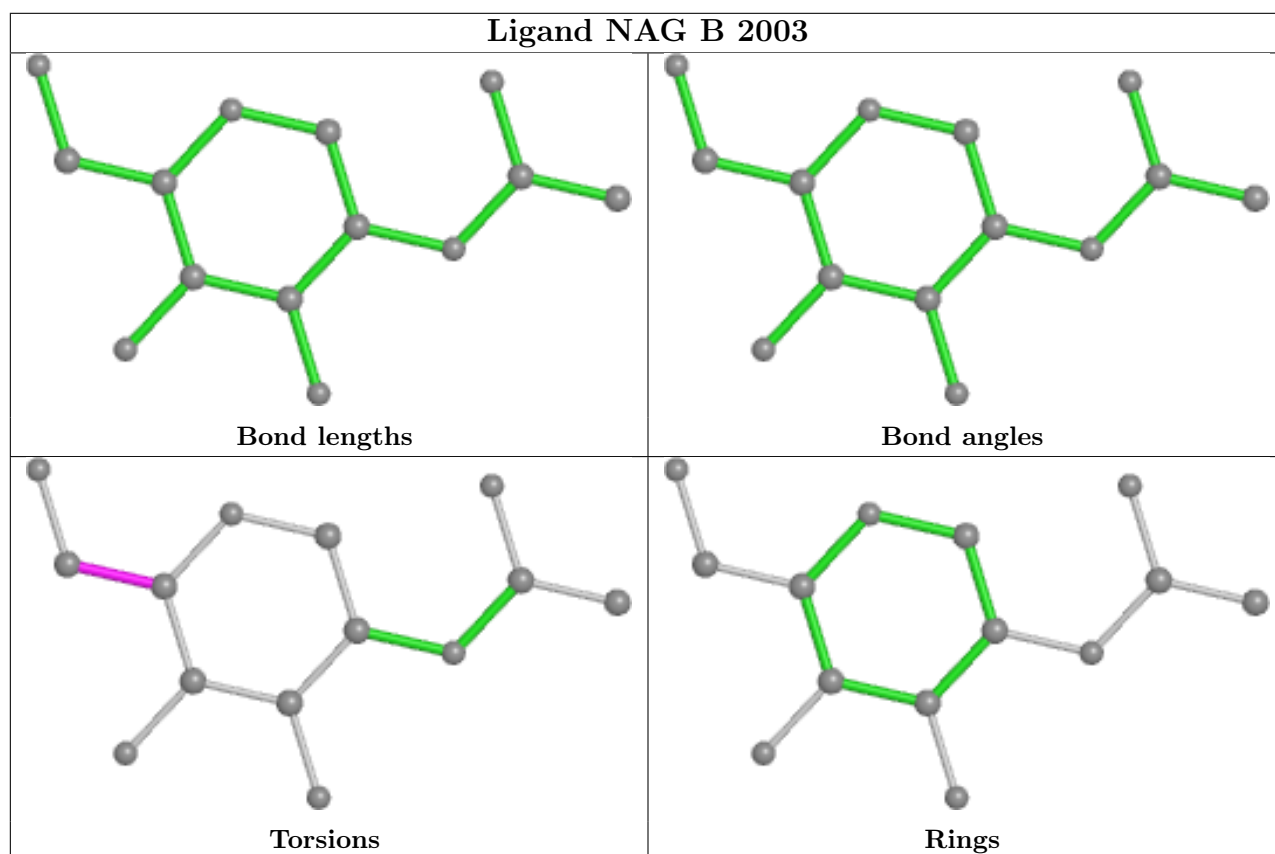
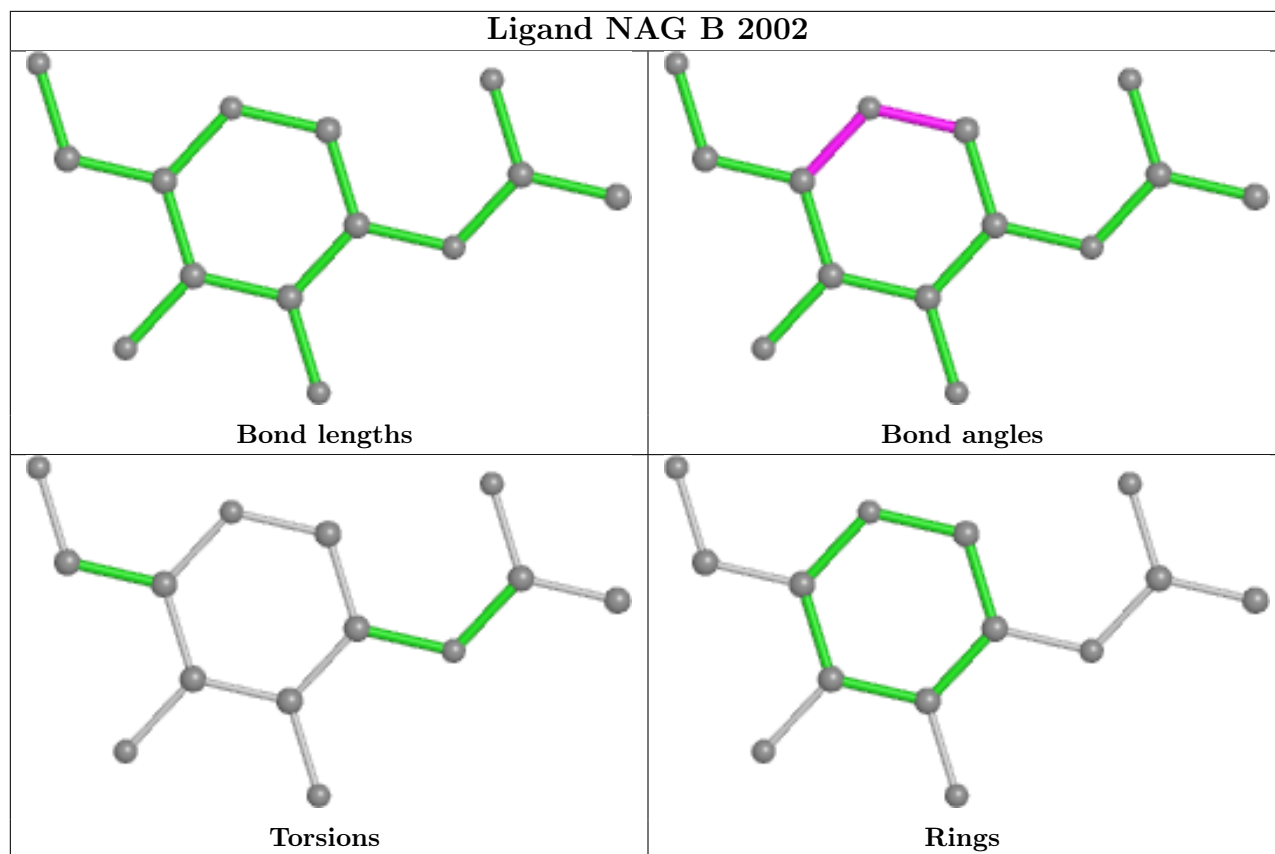




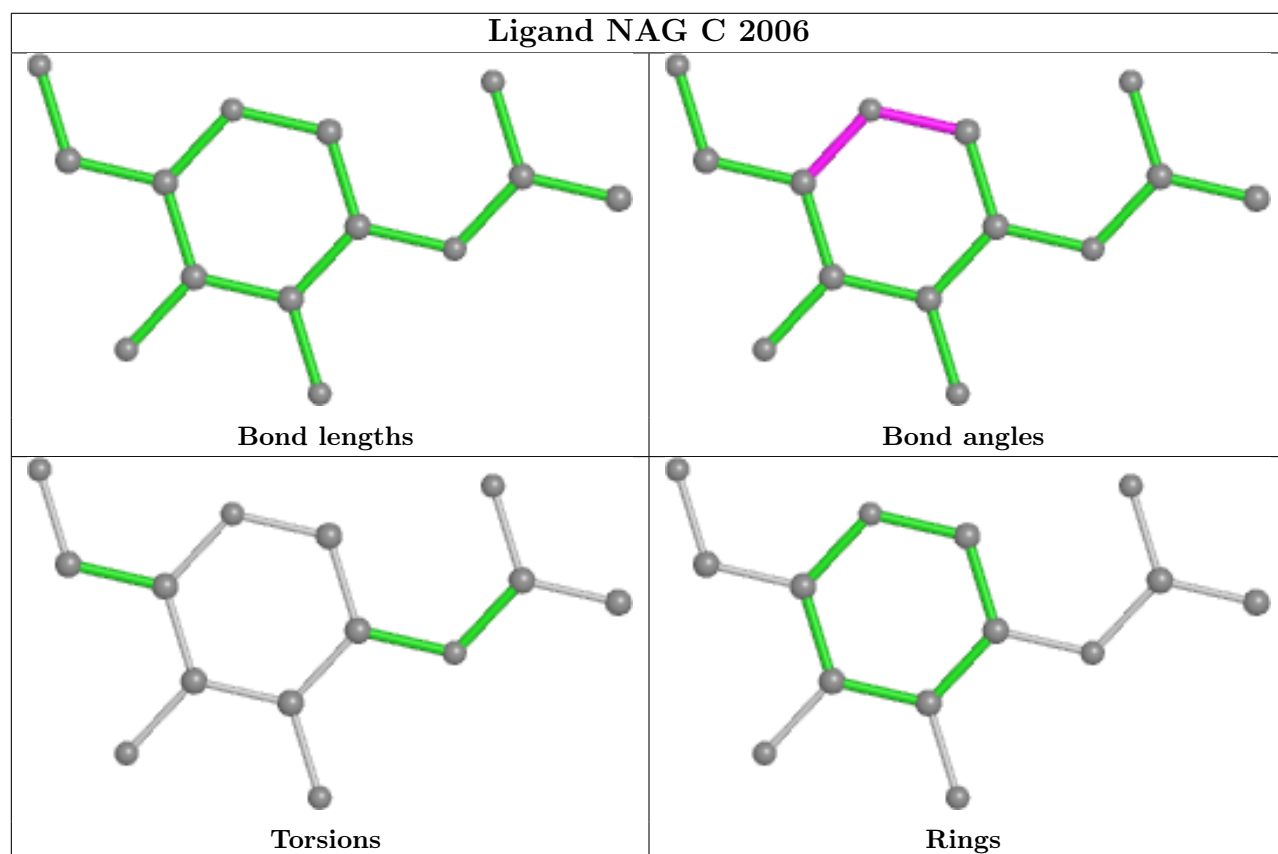
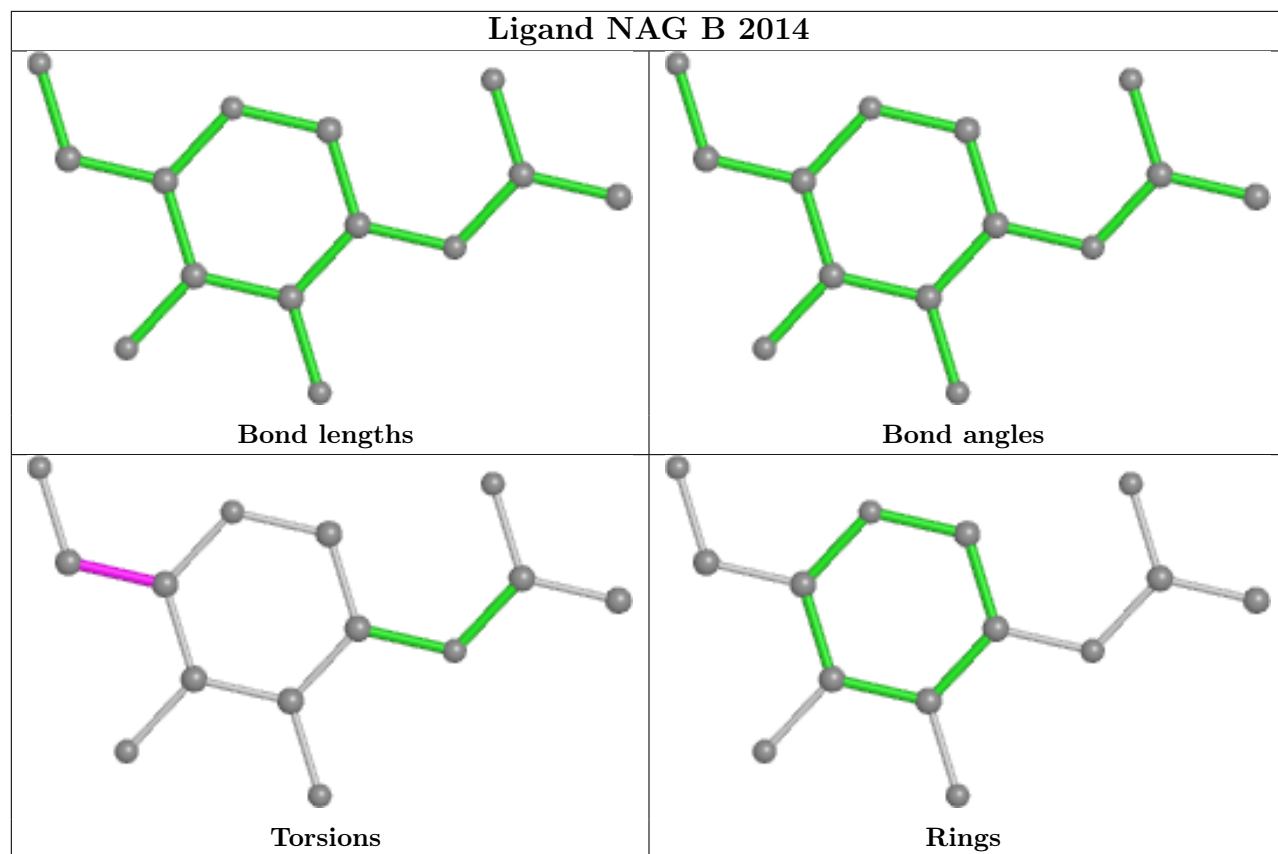


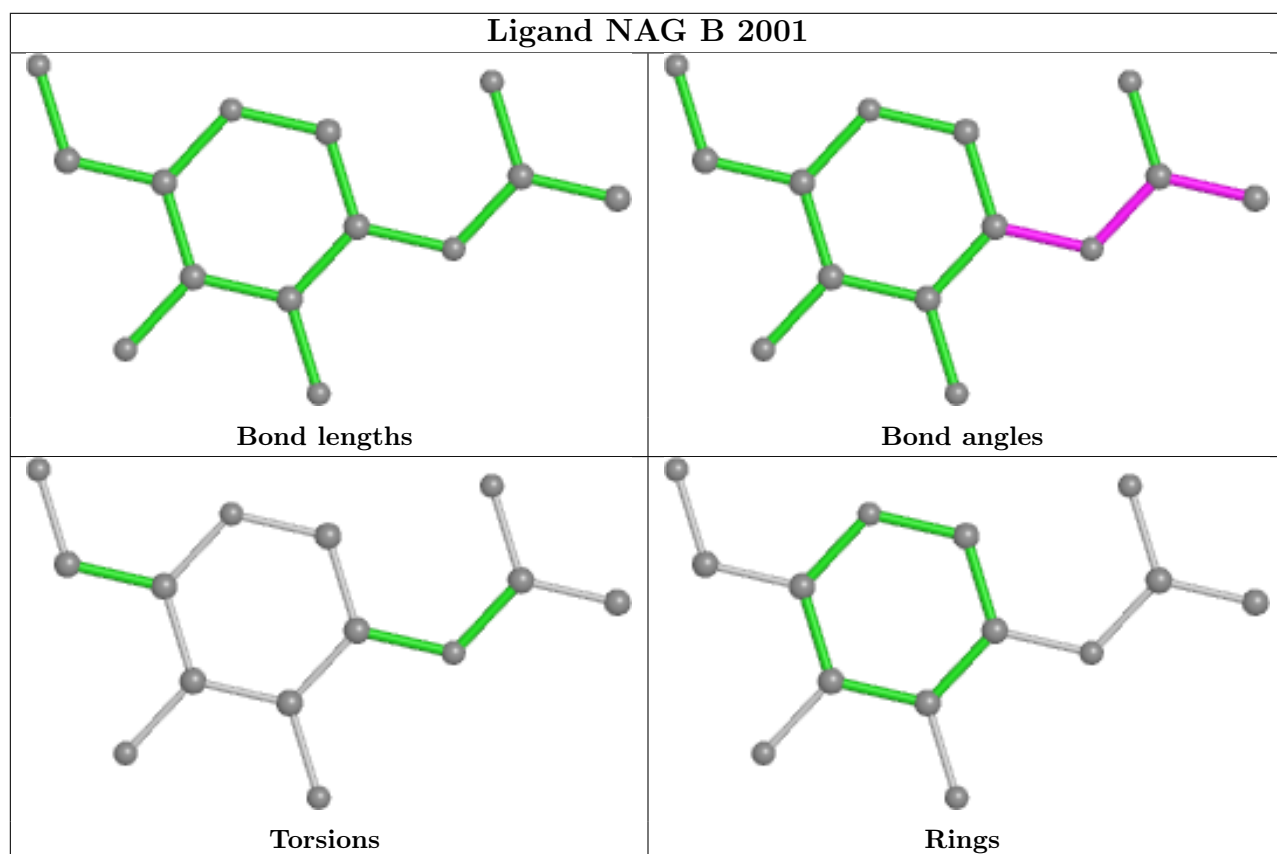
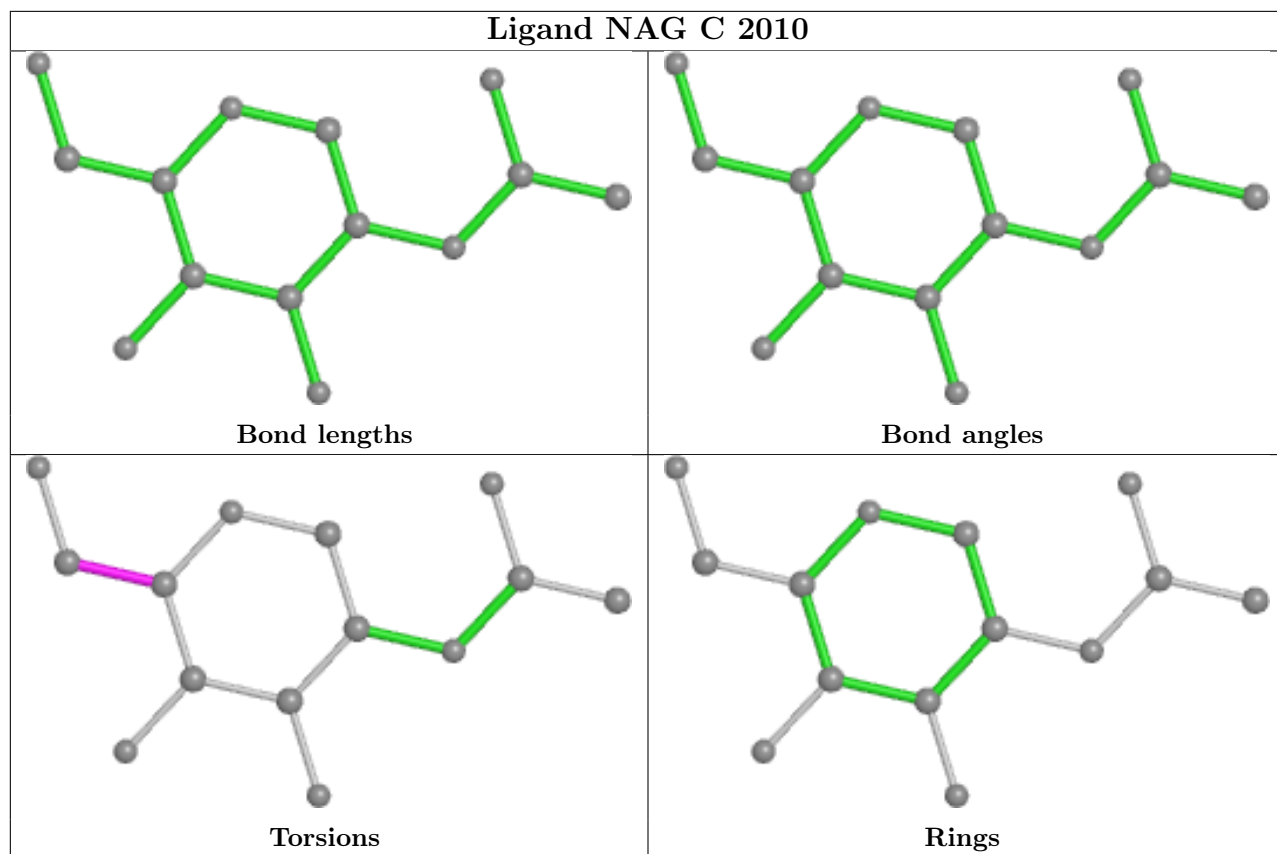


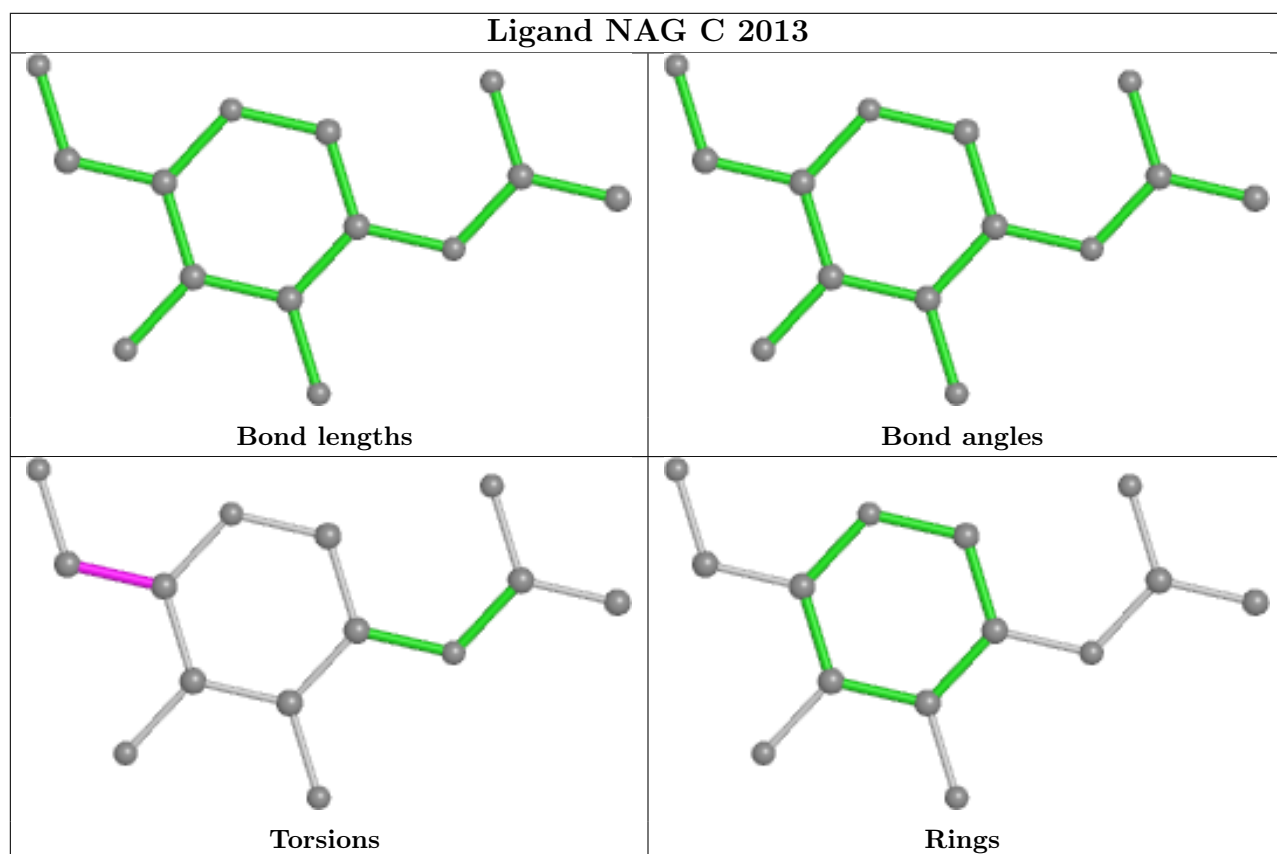
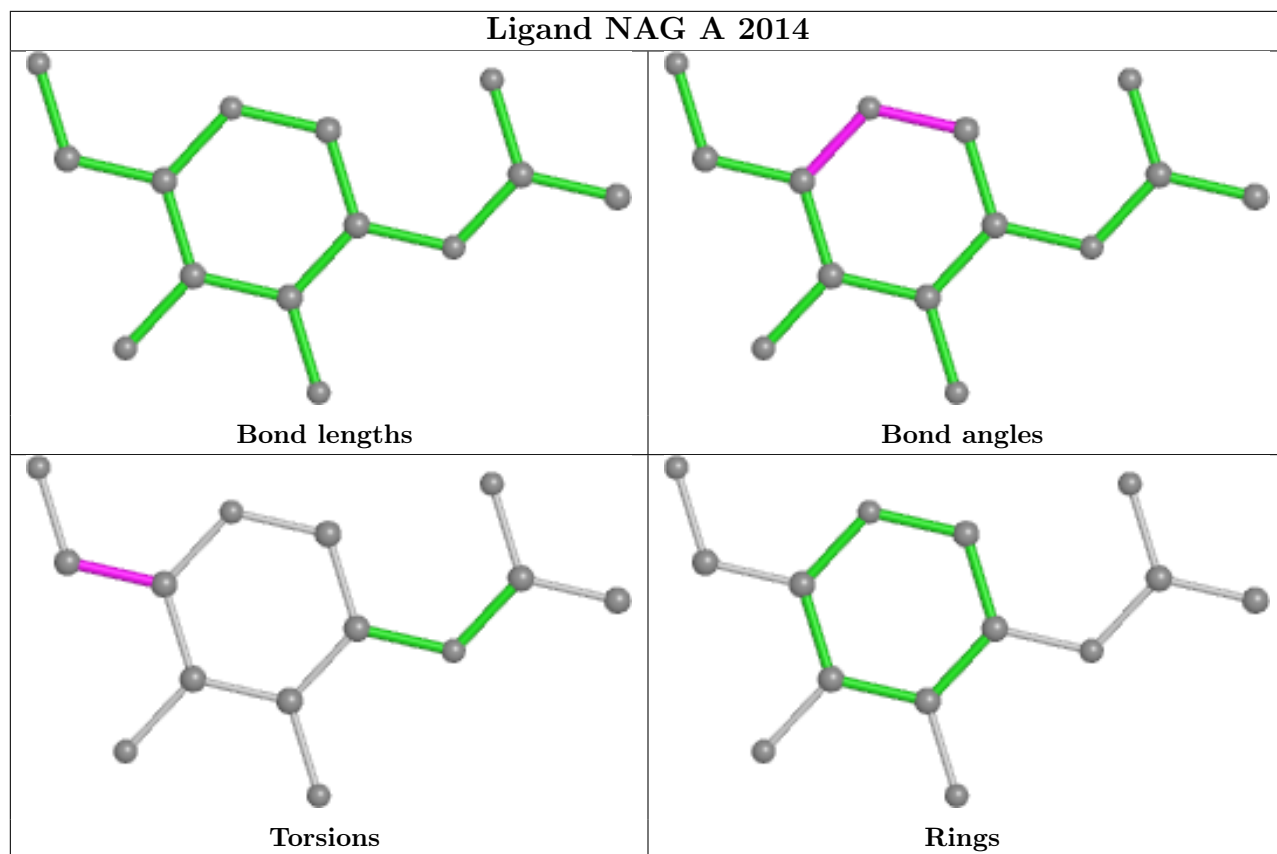


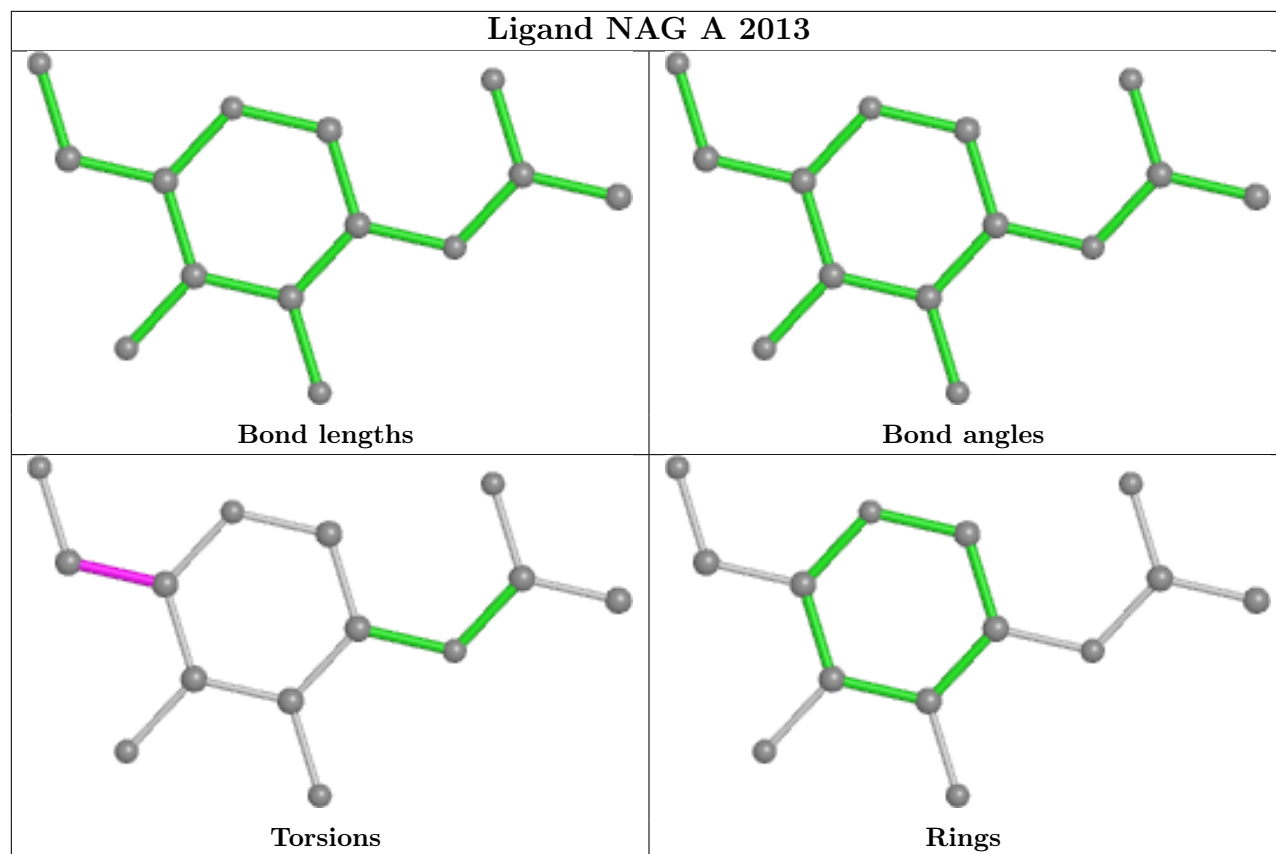












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

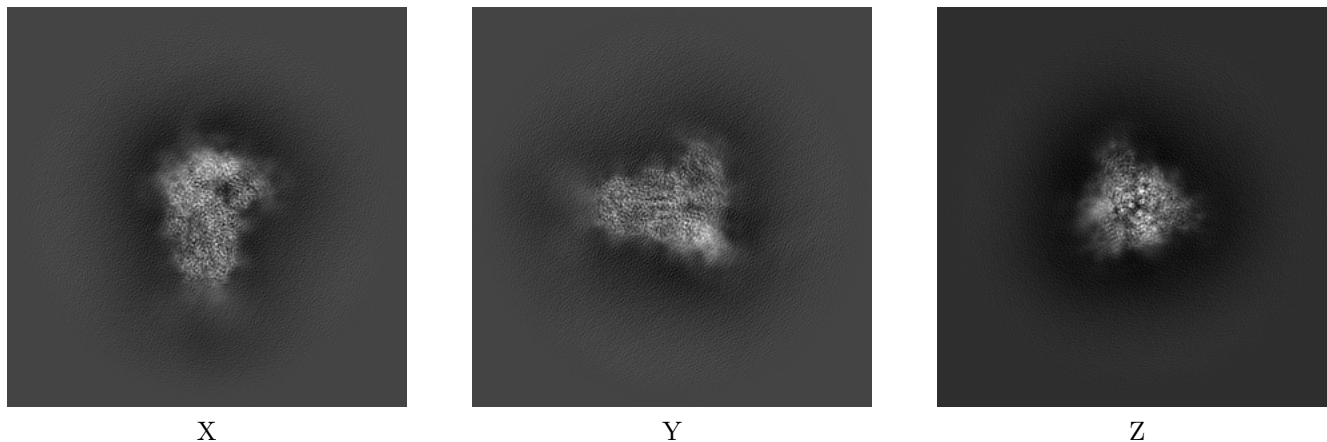
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38829. These allow visual inspection of the internal detail of the map and identification of artifacts.

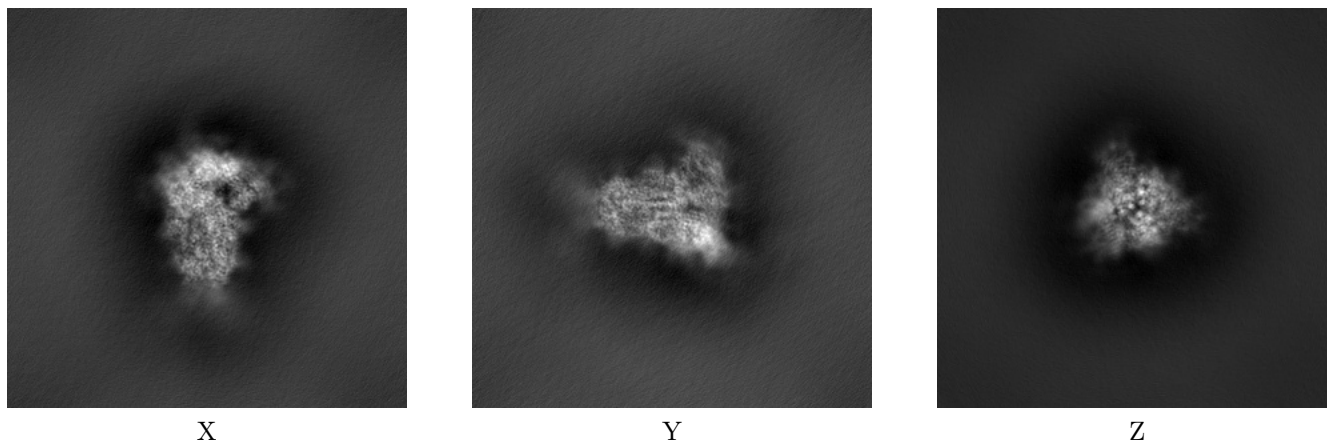
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



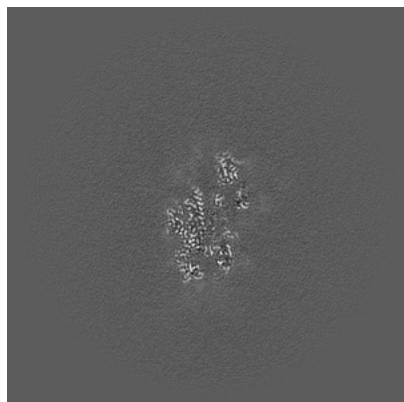
#### 6.1.2 Raw map



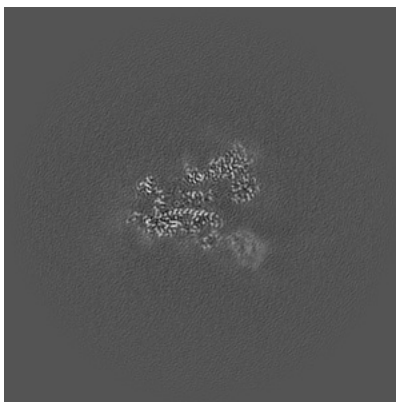
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

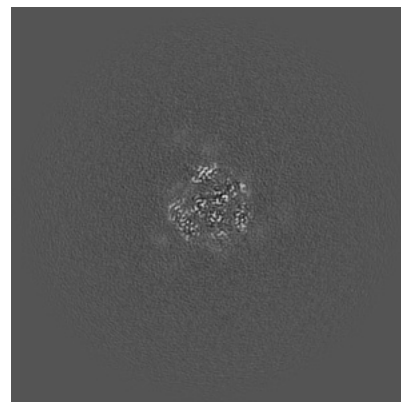
### 6.2.1 Primary map



X Index: 200

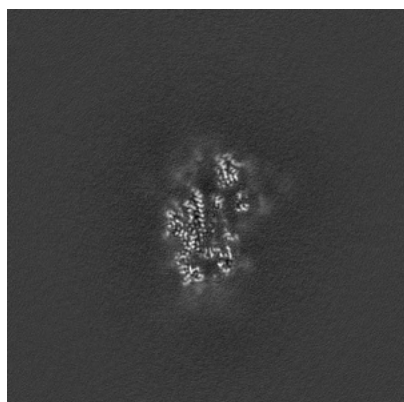


Y Index: 200

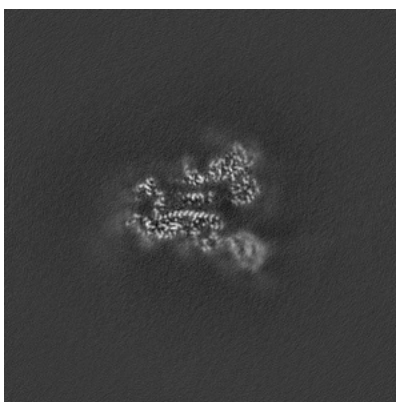


Z Index: 200

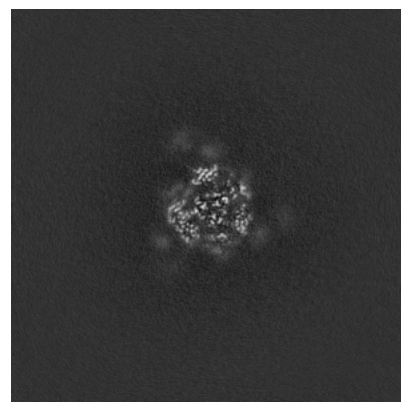
### 6.2.2 Raw map



X Index: 200



Y Index: 200

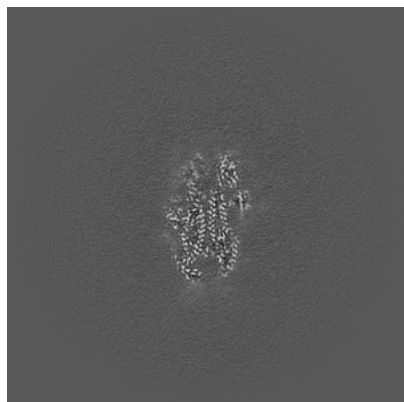


Z Index: 200

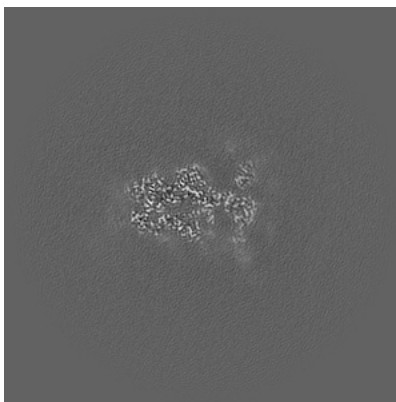
The images above show central slices of the map in three orthogonal directions.

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

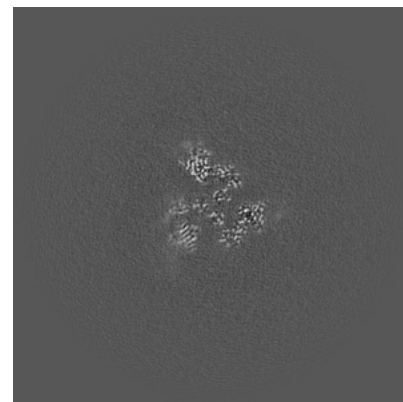
### 6.3.1 Primary map



X Index: 204

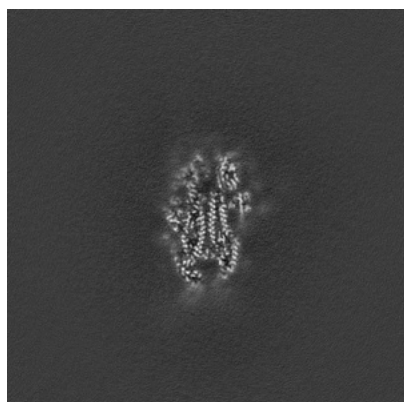


Y Index: 213

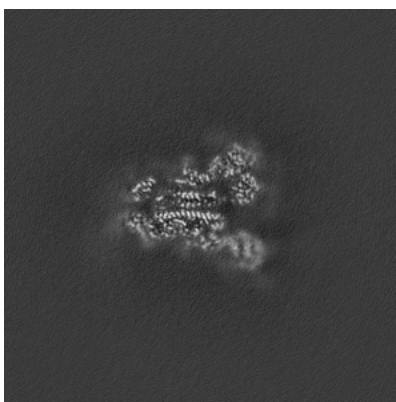


Z Index: 212

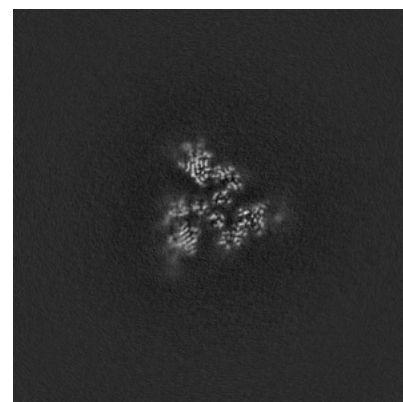
### 6.3.2 Raw map



X Index: 204



Y Index: 202



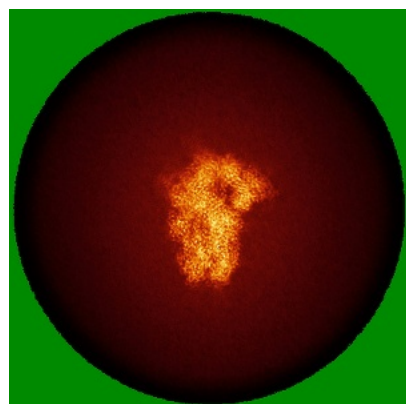
Z Index: 212

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

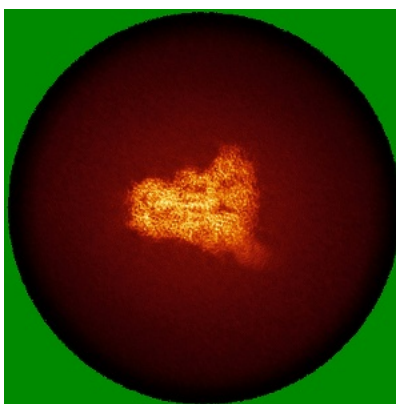


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

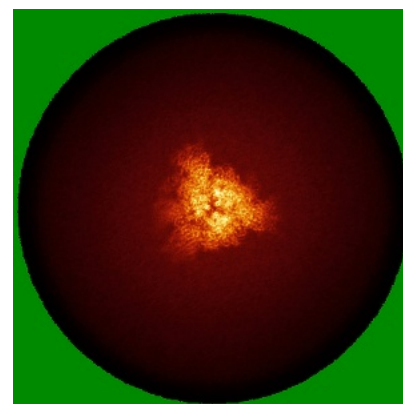
### 6.4.1 Primary map



X



Y

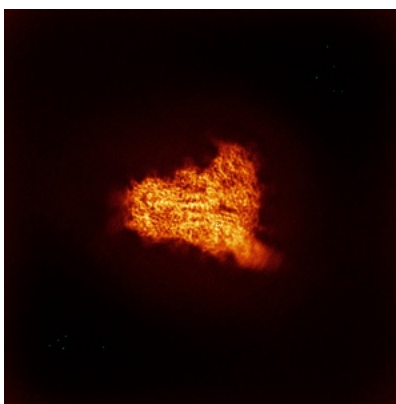


Z

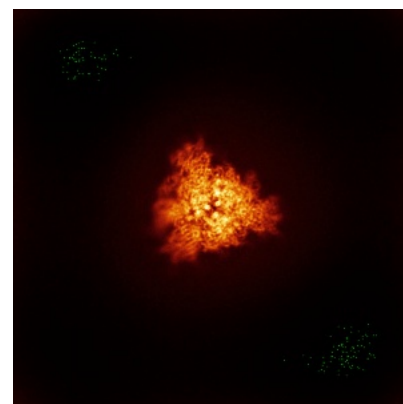
### 6.4.2 Raw map



X



Y



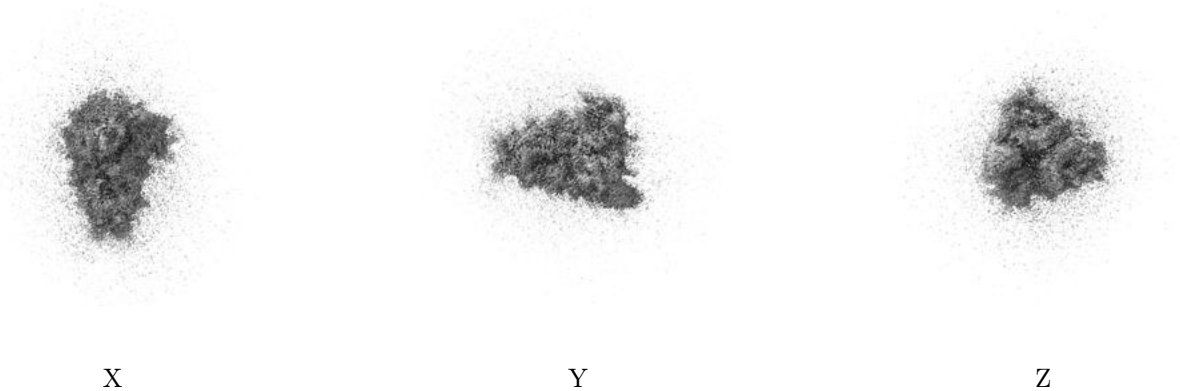
Z

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



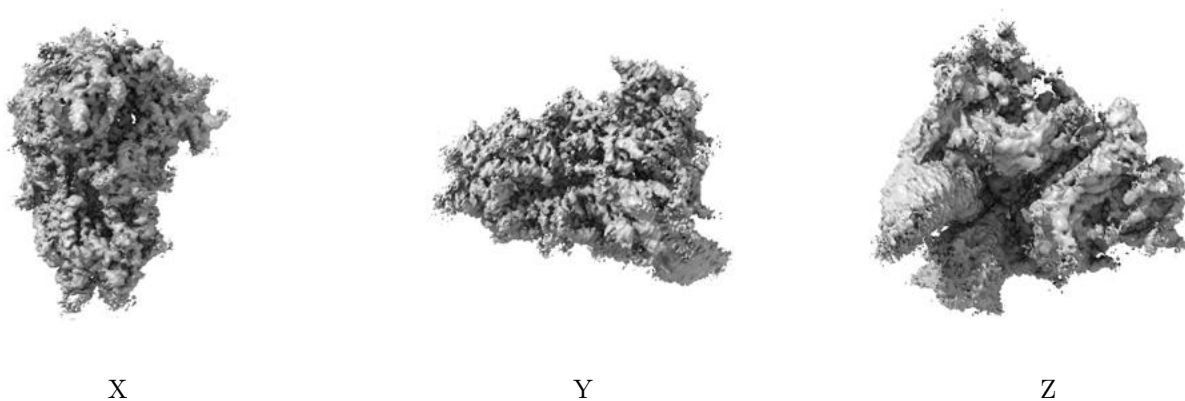
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

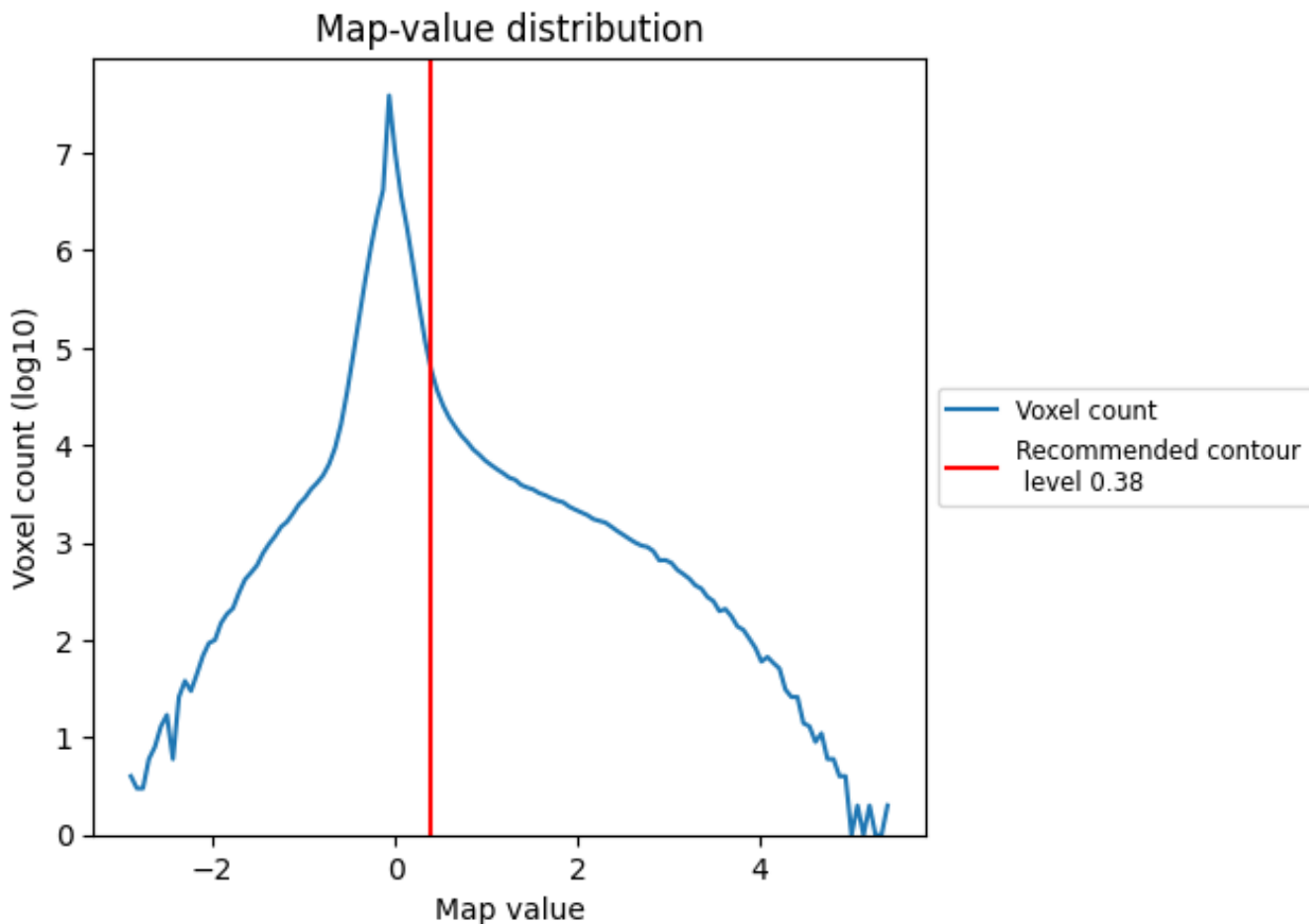
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

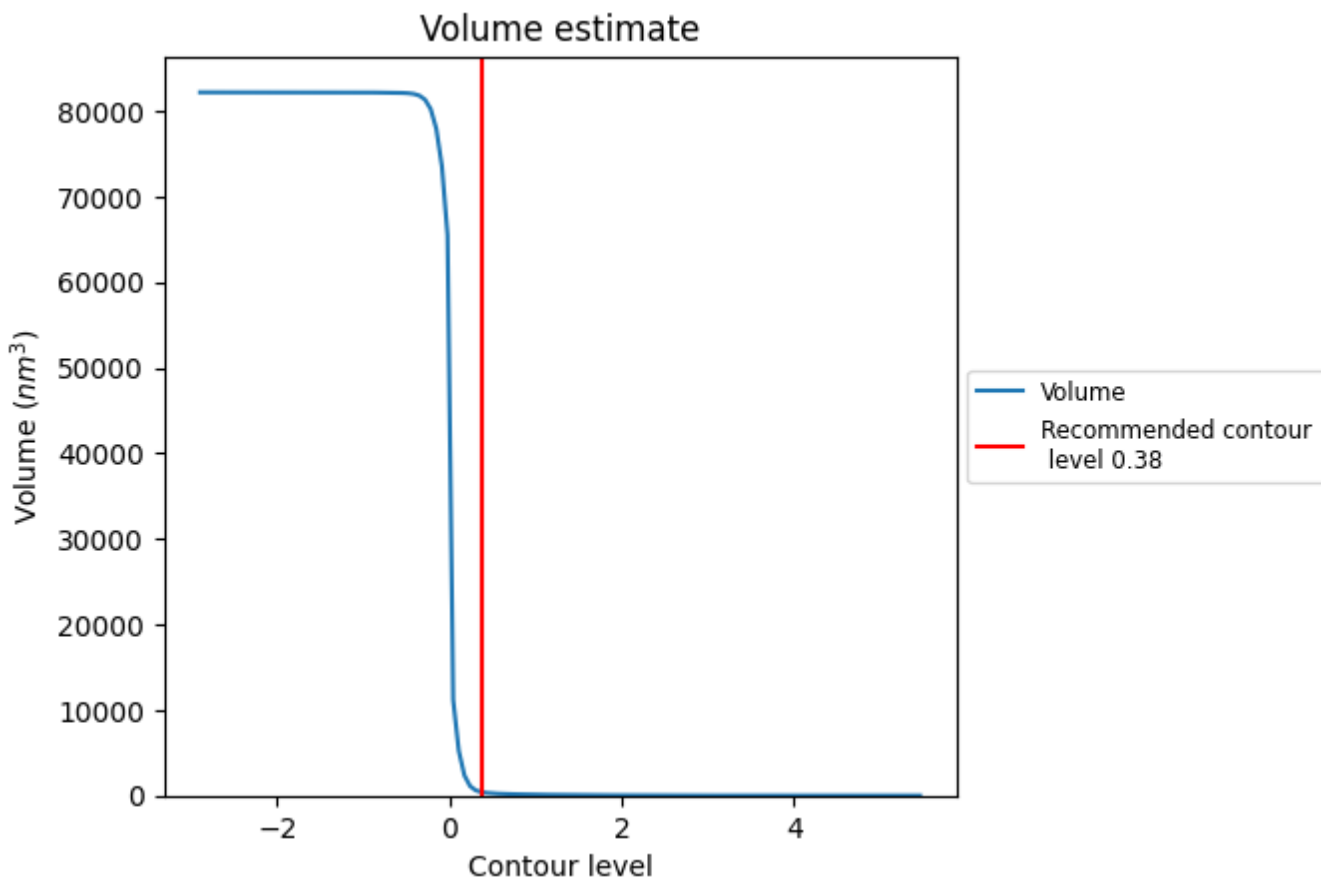
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

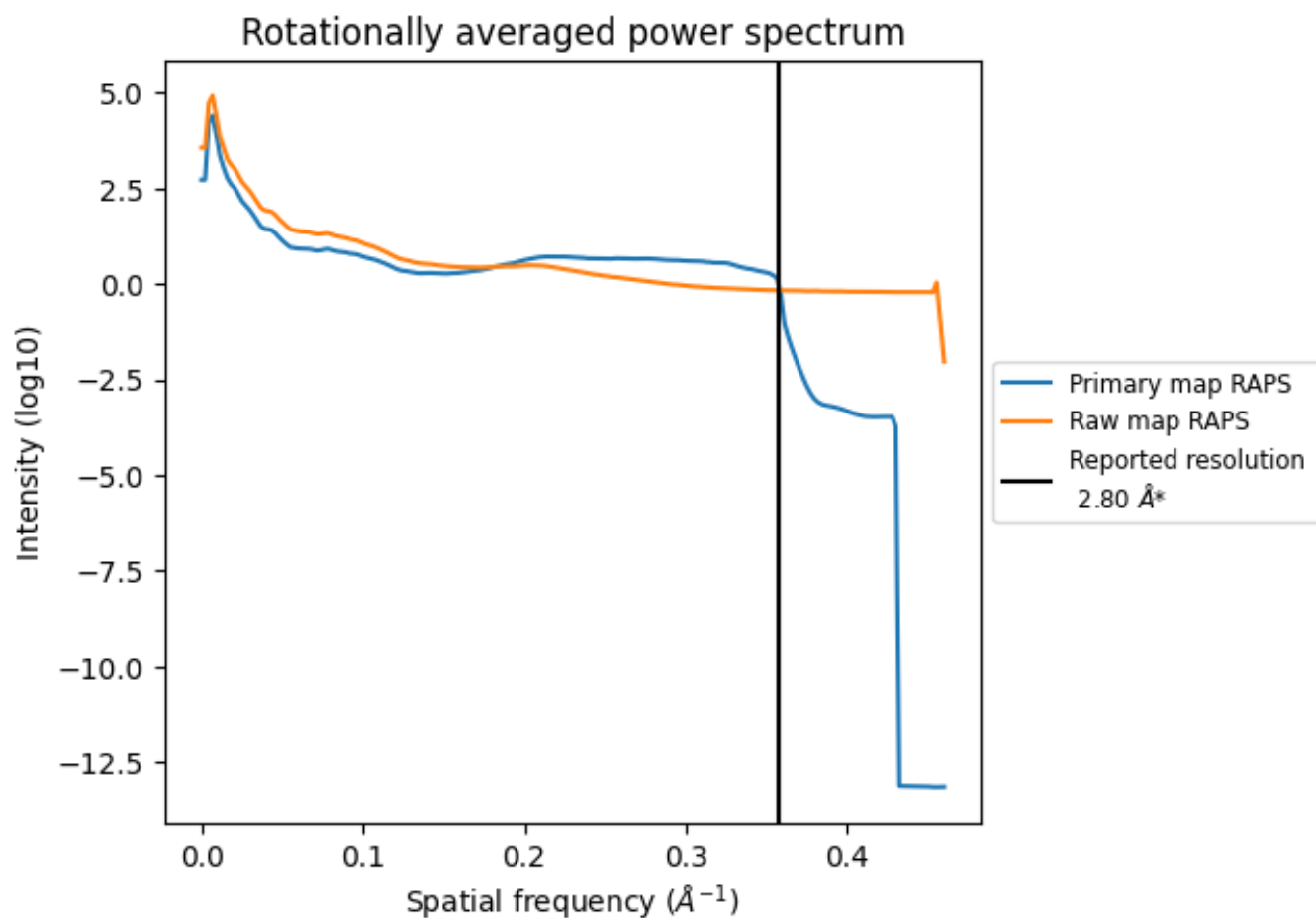
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 394 nm<sup>3</sup>; this corresponds to an approximate mass of 356 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 [i](#)

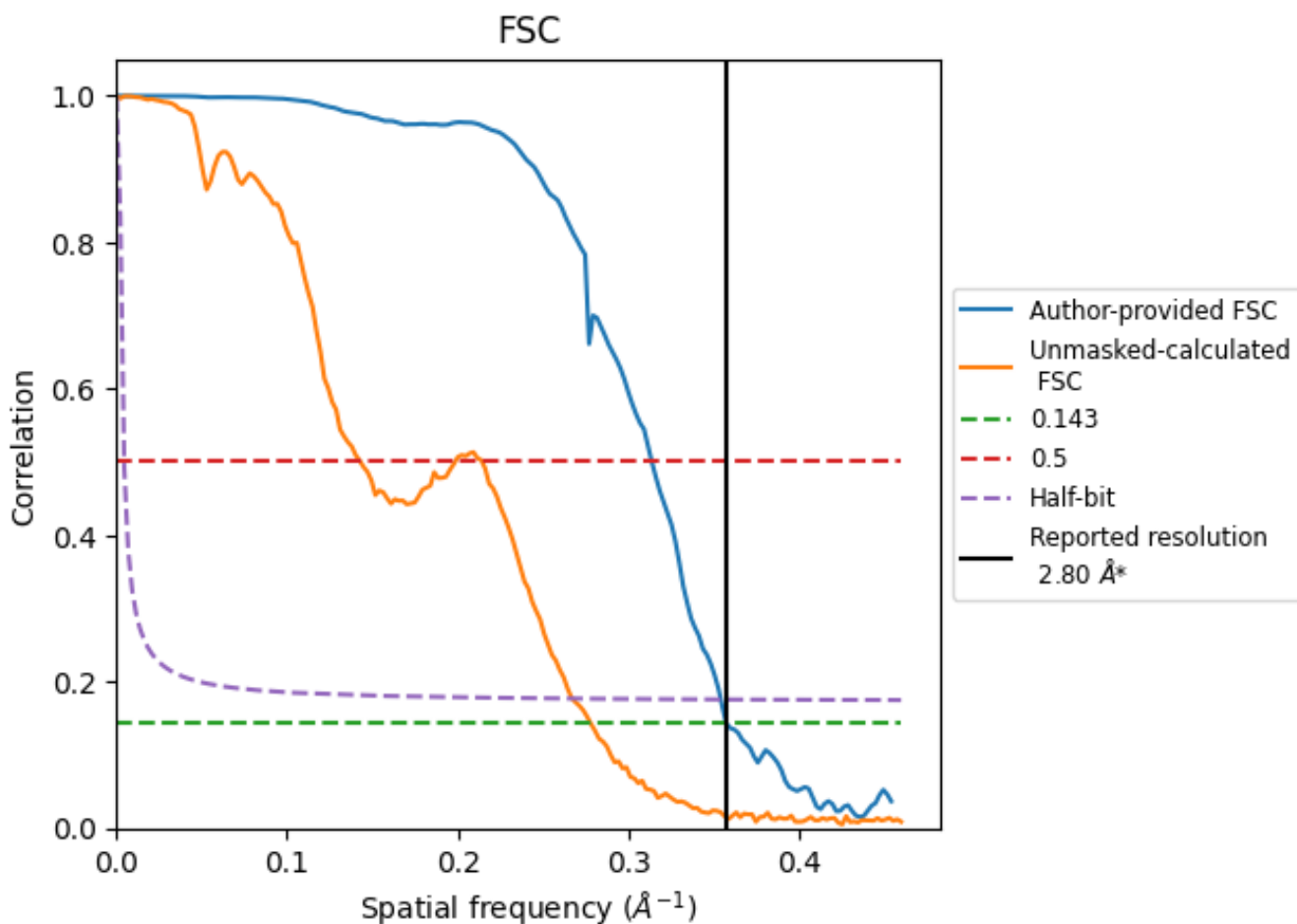


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

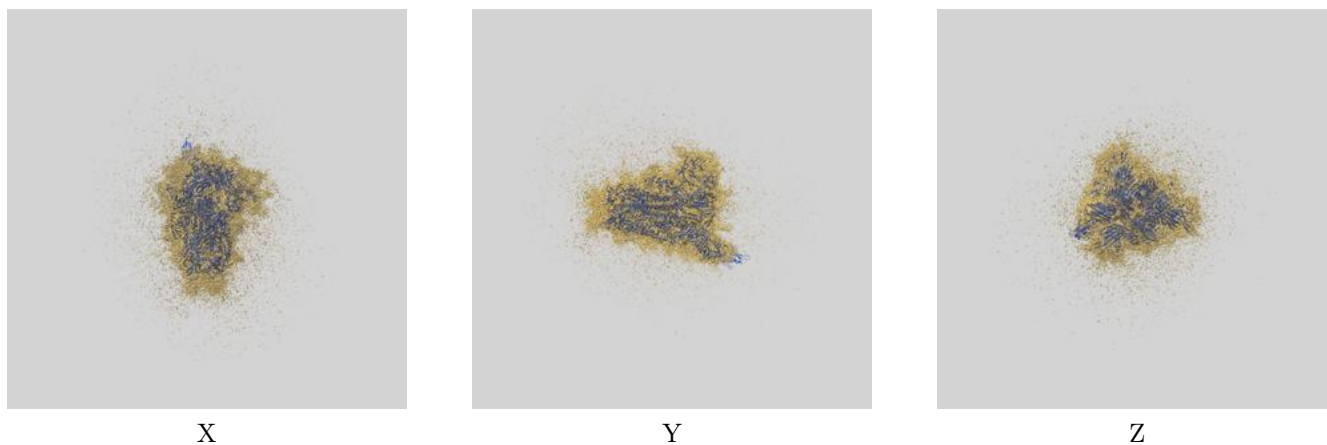
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.19	2.82
Unmasked-calculated*	3.60	6.99	3.74

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.60 differs from the reported value 2.8 by more than 10 %

## 9 Map-model fit [i](#)

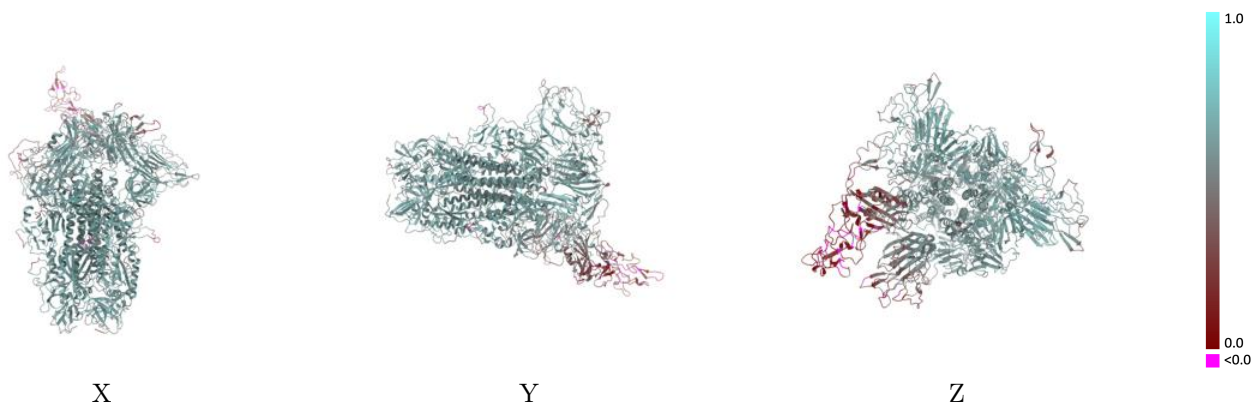
This section contains information regarding the fit between EMDB map EMD-38829 and PDB model 8Y1A. Per-residue inclusion information can be found in section 3 on page 9.

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



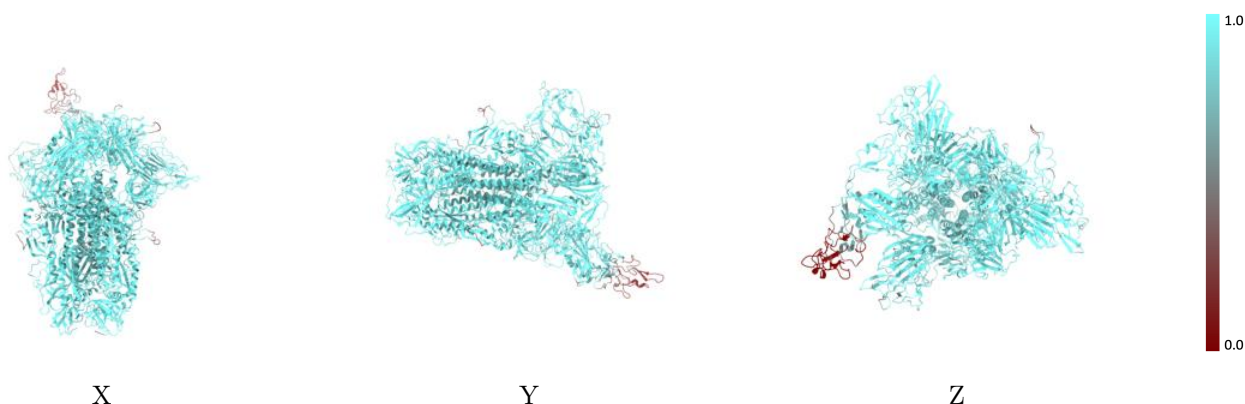
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

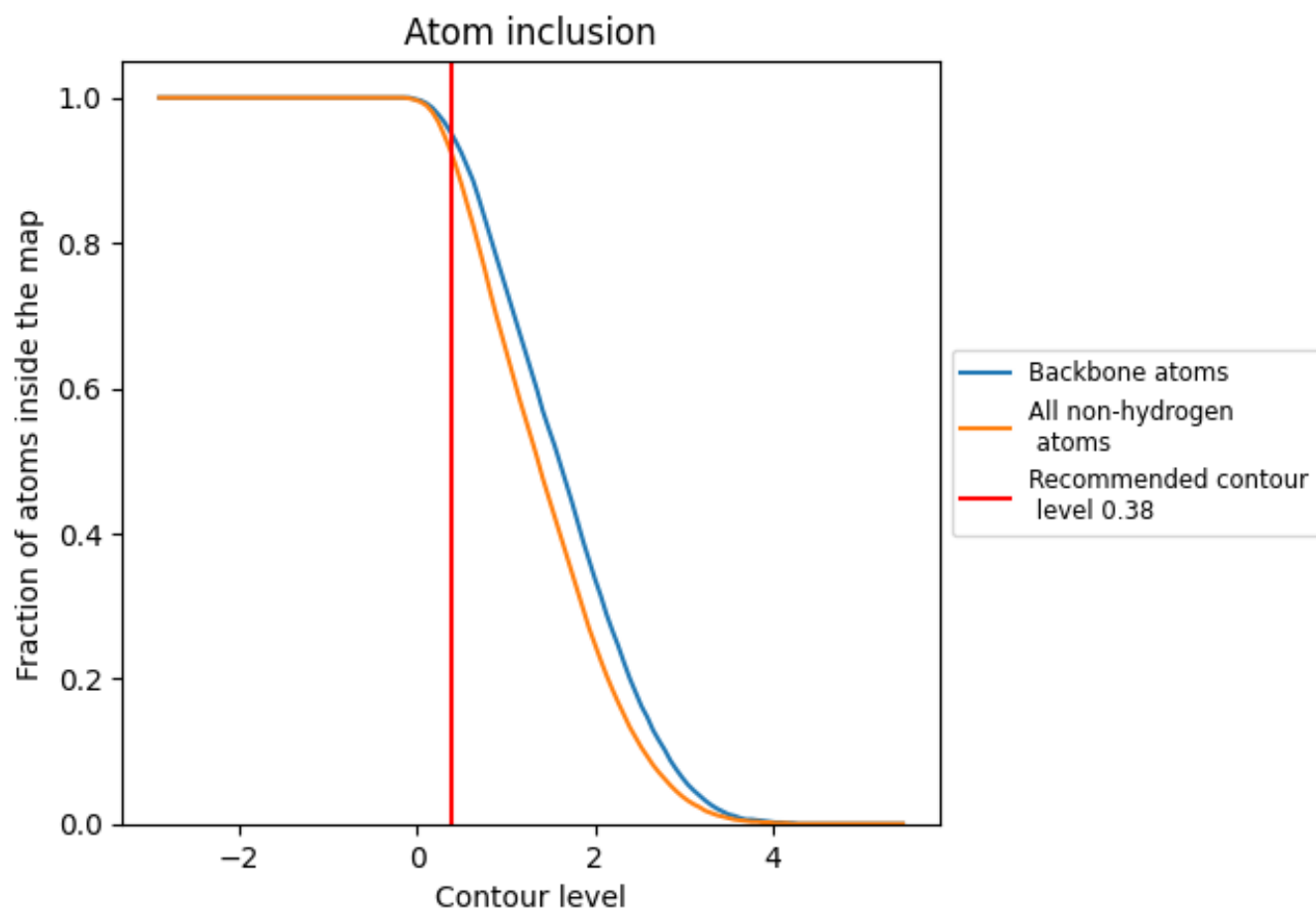
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.38).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9260	 0.5450
A	 0.8820	 0.5070
B	 0.9430	 0.5500
C	 0.9640	 0.5880
D	 0.8890	 0.4610
E	 0.9290	 0.5280
F	 0.5360	 0.2790
G	 0.5000	 0.1990
H	 0.7860	 0.3670
I	 0.3890	 0.1220
J	 0.7860	 0.2180
K	 0.8930	 0.4290
L	 0.2860	 0.3050
M	 0.7500	 0.4820
N	 0.8060	 0.4810
O	 0.9640	 0.5420
P	 0.8570	 0.4640
Q	 0.9640	 0.5490
R	 0.7500	 0.4510

