



Full wwPDB EM Validation Report ⓘ

Oct 21, 2025 – 10:24 PM JST

PDB ID : 9W75 / pdb_00009w75
EMDB ID : EMD-65717
Title : sarbecovirus Rc-o319 S-trimer in a locked-1 conformation
Authors : Wang, J.; Li, Z.X.; Li, Z.M.; Yuan, H.; Xiong, X.
Deposited on : 2025-08-05
Resolution : 2.13 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

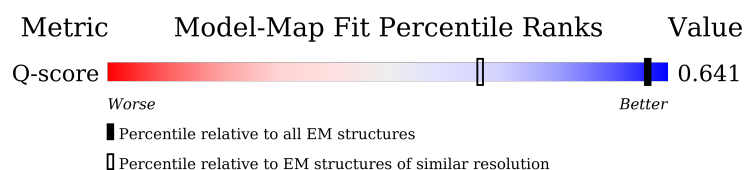
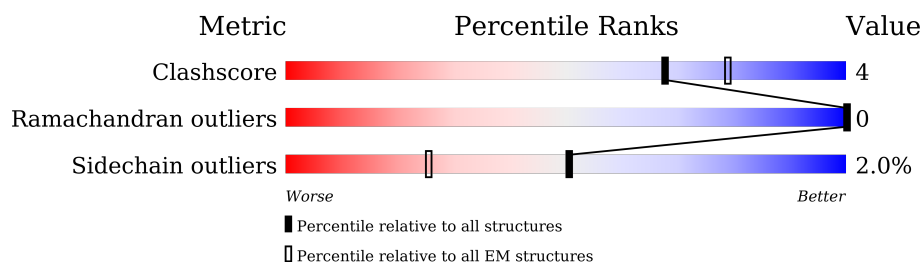
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance

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

The reported resolution of this entry is 2.13 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	2439 (1.64 - 2.63)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1254	 75% 10% 15%
1	B	1254	 76% 9% 15%
1	C	1254	 76% 8% 15%
2	D	2	 100%

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Mol	Chain	Length	Quality of chain
2	E	2	 50% 50%
2	F	2	 100%
2	H	2	 50% 50%
2	I	2	 100%
2	J	2	 50% 50%
2	L	2	 100%
2	M	2	 50% 50%
2	N	2	 50% 50%
2	O	2	 100%
2	Q	2	 100%
3	G	5	 80% 20%
4	K	5	 80% 20%
5	P	4	 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 25997 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 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1061	Total	C	N	O	S	0	0
			8284	5265	1385	1595	39		
1	B	1061	Total	C	N	O	S	0	0
			8284	5265	1385	1595	39		
1	C	1061	Total	C	N	O	S	0	0
			8284	5265	1385	1595	39		

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



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

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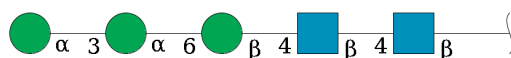
Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-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
3	G	5	Total	C	N	O	0	0
			61	34	2	25		

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



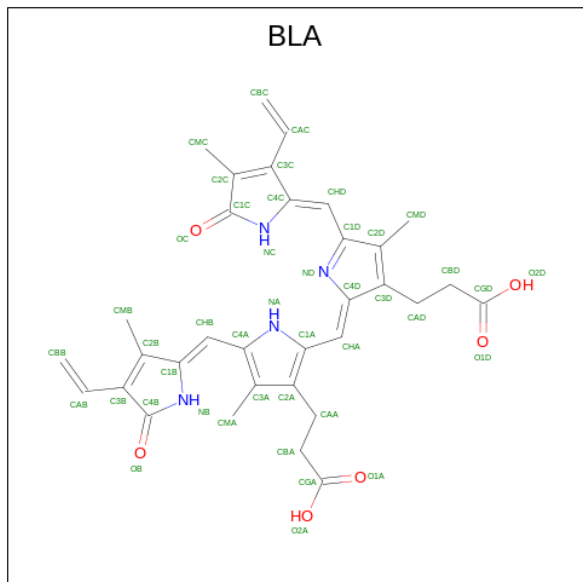
Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



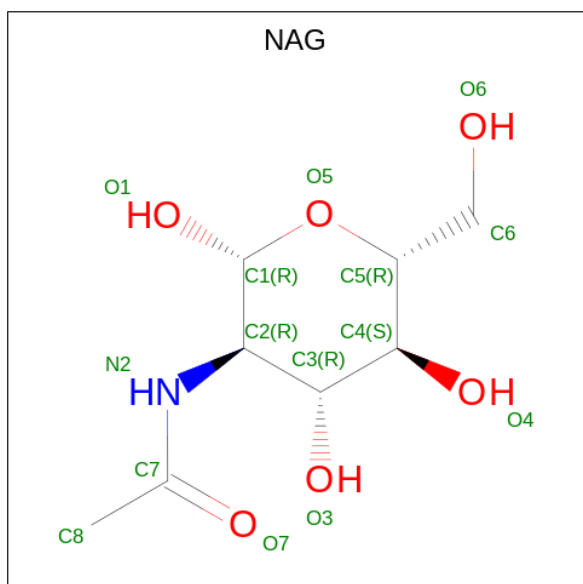
Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is BILIVERDINE IX ALPHA (CCD ID: BLA) (formula: $C_{33}H_{34}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			43	33	4	6	
6	B	1	Total	C	N	O	0
			43	33	4	6	
6	C	1	Total	C	N	O	0
			43	33	4	6	

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



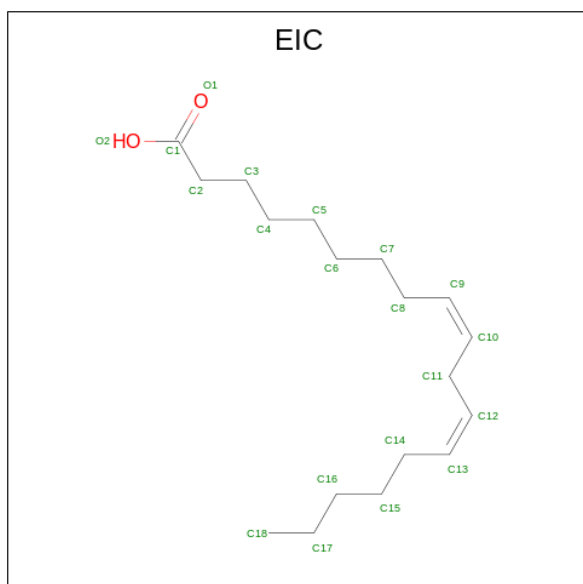
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7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

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

- Molecule 8 is LINOLEIC ACID (CCD ID: EIC) (formula: $C_{18}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).

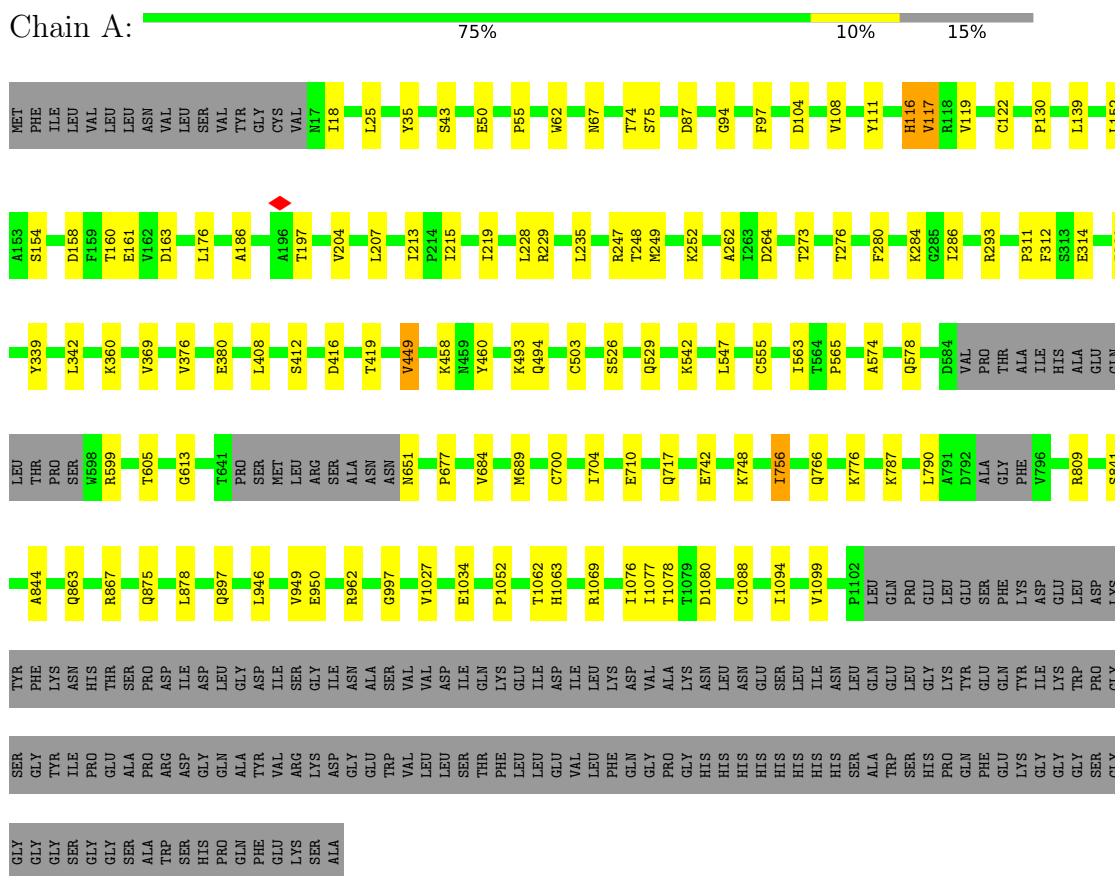


Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total 20	C 18	O 2	0
8	B	1	Total 20	C 18	O 2	0
8	C	1	Total 20	C 18	O 2	0

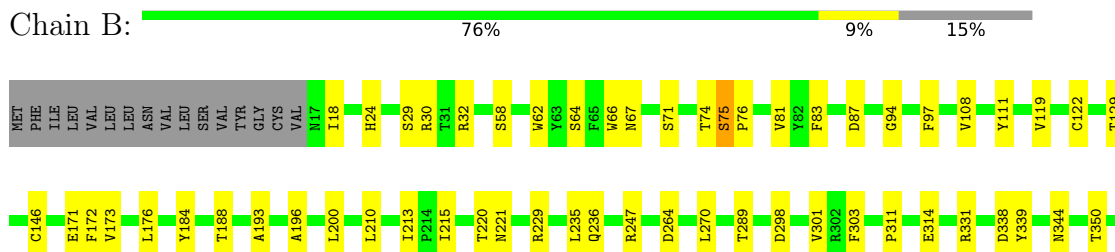
3 Residue-property plots [i](#)

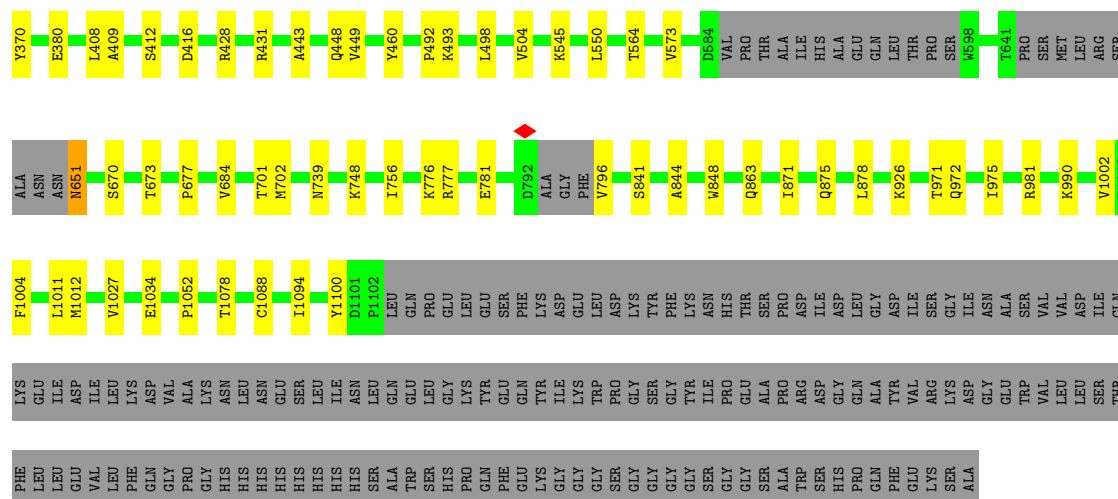
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 protein



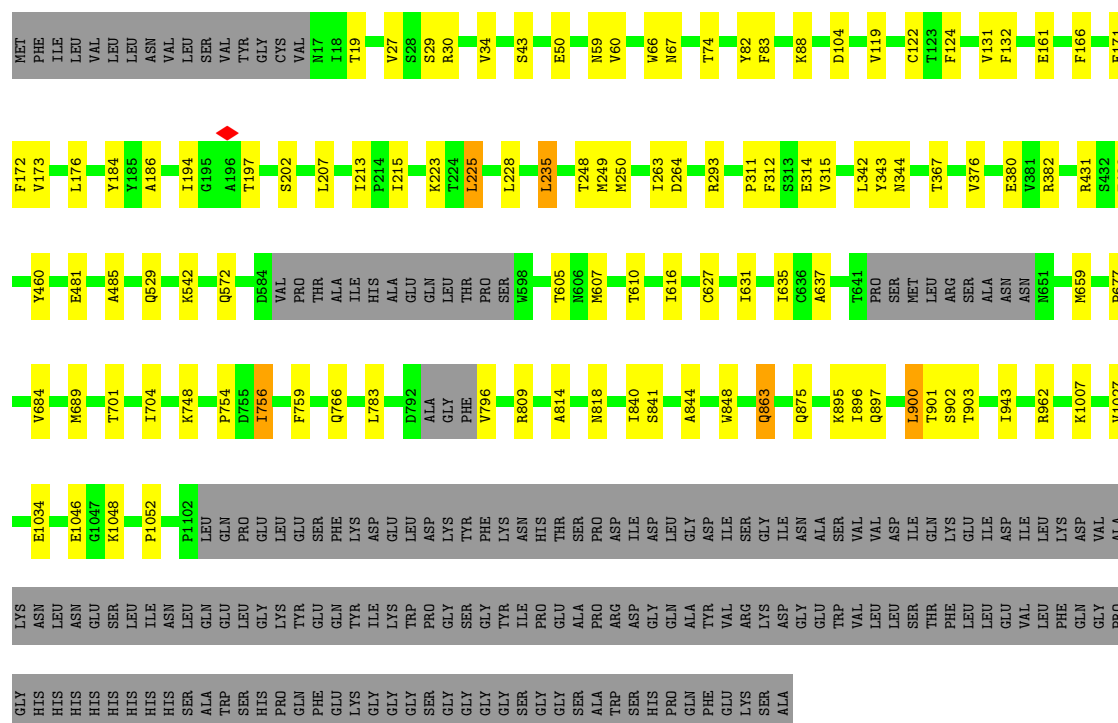
• Molecule 1: Spike protein





• Molecule 1: Spike protein

Chain C: 76% 8% 15%



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

Chain D: 100%



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

Chain E:  50% 50%



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

Chain F:  100%



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

Chain H:  50% 50%




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

Chain I:  100%



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

Chain J:  50% 50%



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

Chain L:  100%



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

Chain M:  50% 50%



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

Chain N:  50% 50%

MAG1
MAG2

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

Chain O:  100%

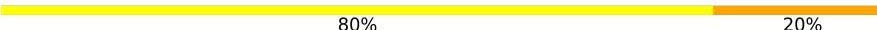
MAG1
MAG2

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

Chain Q:  100%


MAG1
MAG2

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

Chain G:  80% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain K:  80% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

MAG1
MAG2
BMA3
MAN4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	436107	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.932	Depositor
Minimum map value	-0.337	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	297.6, 297.6, 297.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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: BLA, MAN, BMA, NAG, EIC

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	0.14	0/8473	0.36	0/11537
1	B	0.18	0/8473	0.37	0/11537
1	C	0.17	0/8473	0.40	0/11537
All	All	0.16	0/25419	0.38	0/34611

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	8284	0	8017	66	0
1	B	8284	0	8016	64	0
1	C	8284	0	8017	60	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0
2	L	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	28	0	25	0	0
2	N	28	0	25	1	0
2	O	28	0	25	0	0
2	Q	28	0	25	0	0
3	G	61	0	52	1	0
4	K	61	0	52	1	0
5	P	50	0	43	0	0
6	A	43	0	32	1	0
6	B	43	0	32	2	0
6	C	43	0	32	0	0
7	A	154	0	143	0	0
7	B	154	0	143	0	0
7	C	168	0	156	0	0
8	A	20	0	31	1	0
8	B	20	0	31	2	0
8	C	20	0	31	2	0
All	All	25997	0	25103	184	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 (184) 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:B:651:ASN:N	1:B:651:ASN:HD22	1.78	0.80
1:B:651:ASN:N	1:B:651:ASN:ND2	2.38	0.70
1:A:249:MET:HG2	1:A:264:ASP:HA	1.77	0.66
1:C:249:MET:HG2	1:C:264:ASP:HA	1.81	0.62
1:A:1078:THR:HG22	1:A:1080:ASP:H	1.64	0.61
1:A:408:LEU:HD21	8:B:1301:EIC:H51	1.82	0.61
1:A:339:TYR:HB2	8:B:1301:EIC:H61	1.83	0.61
1:C:161:GLU:HG3	1:C:235:LEU:HD13	1.83	0.60
1:A:43:SER:HB2	1:A:809:ARG:HH21	1.66	0.60
1:C:311:PRO:HB2	1:C:314:GLU:HB2	1.84	0.60
1:A:293:ARG:HH22	1:C:701:THR:HB	1.68	0.59
1:B:338:ASP:HA	1:B:492:PRO:HG3	1.86	0.56
1:B:339:TYR:HB2	8:C:1301:EIC:H61	1.88	0.56
1:B:66:TRP:HA	1:B:236:GLN:HA	1.88	0.56
1:A:311:PRO:HB2	1:A:314:GLU:HB2	1.88	0.55
1:A:1052:PRO:O	1:C:875:GLN:NE2	2.39	0.55
1:A:555:CYS:O	1:A:599:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:SER:HB3	1:C:809:ARG:HH21	1.70	0.55
1:C:66:TRP:CD1	1:C:67:ASN:H	2.25	0.55
1:B:220:THR:HG21	4:K:1:NAG:H62	1.88	0.55
1:C:176:LEU:HD11	1:C:215:ILE:HD11	1.89	0.54
1:B:431:ARG:NH2	3:G:1:NAG:O7	2.38	0.54
1:B:119:VAL:HG21	1:B:213:ILE:HG21	1.90	0.54
1:C:131:VAL:HG21	1:C:228:LEU:HD22	1.90	0.54
1:A:284:LYS:HG3	1:A:565:PRO:HA	1.89	0.53
1:A:766:GLN:NE2	1:A:897:GLN:OE1	2.40	0.53
1:A:116:HIS:HB3	1:A:154:SER:HA	1.89	0.53
1:B:303:PHE:O	1:B:545:LYS:NZ	2.40	0.53
1:C:119:VAL:HG21	1:C:213:ILE:HG21	1.91	0.53
1:C:1046:GLU:OE1	1:C:1048:LYS:NZ	2.42	0.53
1:B:301:VAL:HG11	1:B:493:LYS:HG2	1.91	0.53
1:C:902:SER:OG	1:C:903:THR:N	2.41	0.53
1:A:163:ASP:OD1	1:A:163:ASP:N	2.39	0.52
1:B:701:THR:HB	1:C:293:ARG:HH22	1.73	0.52
1:B:841:SER:HA	1:B:844:ALA:HB3	1.90	0.52
1:C:74:THR:HG22	1:C:223:LYS:HD3	1.92	0.52
1:B:176:LEU:HD21	1:B:215:ILE:HD11	1.91	0.52
1:A:161:GLU:HG2	1:A:235:LEU:HD11	1.90	0.52
1:B:32:ARG:NH2	1:B:171:GLU:OE2	2.43	0.52
1:C:610:THR:HB	1:C:635:ILE:HG13	1.92	0.51
1:A:875:GLN:NE2	1:B:1052:PRO:O	2.43	0.51
1:C:704:ILE:O	1:C:962:ARG:NH1	2.42	0.51
1:A:67:ASN:HB3	1:A:229:ARG:HH22	1.75	0.51
1:A:119:VAL:HG21	1:A:213:ILE:HG21	1.93	0.50
1:B:498:LEU:HD21	1:B:550:LEU:HD11	1.92	0.50
1:C:896:ILE:O	1:C:900:LEU:HG	2.11	0.50
1:C:529:GLN:NE2	1:C:542:LYS:O	2.44	0.50
1:B:564:THR:HB	1:B:573:VAL:HG12	1.93	0.50
1:C:27:VAL:HG23	1:C:60:VAL:HG23	1.92	0.50
1:C:607:MET:HG3	1:C:616:ILE:HG12	1.92	0.50
1:A:542:LYS:HE3	1:A:547:LEU:HB3	1.93	0.50
1:C:367:THR:HG21	1:C:485:ALA:HB3	1.93	0.50
1:A:97:PHE:HB2	1:A:108:VAL:HB	1.94	0.50
1:B:875:GLN:NE2	1:C:1052:PRO:O	2.45	0.50
1:C:631:ILE:HD11	1:C:637:ALA:HB2	1.94	0.49
1:B:29:SER:HA	1:B:200:LEU:HD12	1.93	0.49
1:B:311:PRO:HB2	1:B:314:GLU:HG2	1.93	0.49
1:C:841:SER:HA	1:C:844:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:LEU:HD21	8:C:1301:EIC:H51	1.95	0.48
1:A:312:PHE:HB3	1:A:342:LEU:HD21	1.95	0.48
1:B:122:CYS:HA	1:B:146:CYS:HA	1.95	0.48
1:B:193:ALA:HB3	1:B:196:ALA:HB2	1.95	0.48
1:B:97:PHE:HB2	1:B:108:VAL:HB	1.95	0.48
1:C:627:CYS:HB2	1:C:659:MET:HE3	1.96	0.48
1:C:50:GLU:HB2	1:C:248:THR:HG23	1.95	0.48
1:B:670:SER:OG	1:B:673:THR:OG1	2.30	0.48
1:C:677:PRO:HA	1:C:1034:GLU:HA	1.95	0.48
1:B:871:ILE:HD13	1:B:1011:LEU:HD21	1.95	0.47
1:A:503:CYS:HB2	1:A:555:CYS:HB3	1.80	0.47
1:B:684:VAL:HG22	1:B:1027:VAL:HG22	1.95	0.47
1:A:412:SER:OG	1:A:416:ASP:OD1	2.29	0.47
1:C:186:ALA:HB2	1:C:207:LEU:HA	1.97	0.47
1:A:360:LYS:NZ	1:C:943:ILE:O	2.47	0.47
1:A:841:SER:HA	1:A:844:ALA:HB3	1.95	0.47
1:B:74:THR:HG22	1:B:221:ASN:HB3	1.97	0.47
1:C:122:CYS:HB2	1:C:124:PHE:CZ	2.49	0.47
2:E:1:NAG:H83	2:E:1:NAG:H3	1.96	0.47
1:B:428:ARG:NH2	1:B:443:ALA:O	2.46	0.47
1:B:122:CYS:HB3	1:B:146:CYS:HB2	1.70	0.46
1:C:814:ALA:O	1:C:818:ASN:ND2	2.49	0.46
1:C:380:GLU:OE1	1:C:460:TYR:OH	2.31	0.46
1:A:689:MET:HE2	1:A:689:MET:HB3	1.80	0.46
1:B:298:ASP:HB2	1:B:504:VAL:HG12	1.97	0.46
1:C:689:MET:HE2	1:C:689:MET:HB3	1.78	0.46
1:B:18:ILE:HD12	1:B:129:THR:HG21	1.97	0.46
1:B:173:VAL:HB	1:B:184:TYR:HB2	1.98	0.46
1:A:529:GLN:NE2	1:A:542:LYS:O	2.49	0.45
1:B:990:LYS:NZ	1:B:1004:PHE:O	2.49	0.45
1:A:787:LYS:HA	1:A:787:LYS:HD3	1.80	0.45
1:A:1069:ARG:HD3	1:C:848:TRP:HZ2	1.80	0.45
1:C:431:ARG:NH1	1:C:433:GLU:O	2.49	0.45
1:A:158:ASP:HB3	1:A:160:THR:HG23	1.99	0.45
1:A:273:THR:HA	1:A:276:THR:HG22	1.99	0.45
1:C:766:GLN:NE2	1:C:897:GLN:OE1	2.50	0.45
1:A:684:VAL:HG22	1:A:1027:VAL:HG22	1.98	0.45
1:A:756:ILE:H	1:A:756:ILE:HG13	1.53	0.45
1:B:29:SER:OG	1:B:58:SER:OG	2.33	0.45
1:B:350:THR:HB	1:B:409:ALA:HB3	1.99	0.45
1:A:563:ILE:HB	1:A:574:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:SER:O	1:B:71:SER:OG	2.36	0.44
1:B:677:PRO:HA	1:B:1034:GLU:HA	1.99	0.44
1:B:971:THR:O	1:B:975:ILE:HG12	2.18	0.44
1:C:312:PHE:HB3	1:C:342:LEU:HD21	2.00	0.44
1:C:88:LYS:HB3	1:C:166:PHE:HA	2.00	0.44
1:C:684:VAL:HG22	1:C:1027:VAL:HG22	2.00	0.44
1:A:97:PHE:HB3	1:A:219:ILE:HD13	1.99	0.44
1:A:204:VAL:HG21	1:A:262:ALA:H	1.82	0.44
1:A:252:LYS:HB2	1:A:280:PHE:CE1	2.53	0.44
1:B:94:GLY:HA3	1:B:111:TYR:HA	2.00	0.44
1:B:83:PHE:HB3	1:B:172:PHE:HB2	2.00	0.44
1:A:130:PRO:HB3	1:A:139:LEU:HA	1.99	0.43
1:B:848:TRP:HZ3	1:B:863:GLN:HG3	1.83	0.43
6:B:1302:BLA:HA	6:B:1302:BLA:HB	1.65	0.43
1:A:677:PRO:HA	1:A:1034:GLU:HA	1.99	0.43
1:A:997:GLY:HA3	1:B:1002:VAL:HG21	2.00	0.43
1:B:875:GLN:H	1:B:875:GLN:HG2	1.56	0.43
1:B:24:HIS:HA	1:B:62:TRP:O	2.18	0.43
1:C:104:ASP:OD1	1:C:104:ASP:N	2.52	0.43
1:A:176:LEU:HD21	1:A:215:ILE:HD11	2.00	0.43
1:B:926:LYS:HE3	1:B:926:LYS:HB2	1.78	0.43
1:A:55:PRO:HG3	1:A:247:ARG:HD2	2.01	0.43
1:C:30:ARG:HH22	1:C:202:SER:HB3	1.84	0.43
1:B:1012:MET:HB2	1:B:1027:VAL:HB	2.00	0.43
1:B:1078:THR:HG22	1:B:1100:TYR:HB3	2.01	0.43
1:C:173:VAL:HB	1:C:184:TYR:HB2	2.01	0.43
1:B:247:ARG:NH1	1:B:264:ASP:OD2	2.52	0.43
1:B:1088:CYS:HB2	1:B:1094:ILE:HD13	2.00	0.43
1:A:748:LYS:HD2	1:A:748:LYS:HA	1.74	0.42
1:A:104:ASP:N	1:A:104:ASP:OD1	2.51	0.42
1:A:863:GLN:O	1:A:867:ARG:HG2	2.19	0.42
1:B:412:SER:OG	1:B:416:ASP:OD2	2.32	0.42
1:B:739:ASN:OD1	1:B:981:ARG:NH1	2.42	0.42
1:A:449:VAL:HG22	2:N:2:NAG:H83	2.01	0.42
1:A:25:LEU:HB3	1:A:62:TRP:HB3	2.02	0.42
1:B:748:LYS:HA	1:B:748:LYS:HD2	1.87	0.42
1:C:631:ILE:HD12	1:C:635:ILE:HG22	2.01	0.42
1:A:776:LYS:HD3	1:A:776:LYS:HA	1.69	0.42
1:C:783:LEU:HD13	1:C:900:LEU:HD12	2.01	0.42
1:A:25:LEU:HD12	1:A:25:LEU:HA	1.91	0.42
1:B:344:ASN:HB2	2:J:1:NAG:H83	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLU:OE1	1:A:460:TYR:OH	2.34	0.42
1:B:210:LEU:HD21	6:B:1302:BLA:HHB	2.01	0.42
1:B:777:ARG:HB3	1:B:781:GLU:HB3	2.02	0.42
1:C:82:TYR:OH	1:C:171:GLU:OE2	2.38	0.42
1:A:94:GLY:HA3	1:A:111:TYR:HA	2.02	0.42
1:A:458:LYS:NZ	1:C:344:ASN:O	2.53	0.42
1:A:1077:ILE:HG22	1:A:1099:VAL:HG13	2.02	0.42
1:C:176:LEU:HD12	1:C:176:LEU:HA	1.91	0.42
1:A:87:ASP:N	1:A:87:ASP:OD1	2.53	0.41
1:A:18:ILE:HD11	1:A:228:LEU:HD11	2.02	0.41
1:A:35:TYR:HA	1:A:207:LEU:H	1.85	0.41
1:C:83:PHE:HB3	1:C:172:PHE:HB2	2.01	0.41
1:A:50:GLU:HB2	1:A:248:THR:HG23	2.02	0.41
1:A:704:ILE:O	1:A:962:ARG:NH1	2.46	0.41
8:A:1313:EIC:H21	1:C:343:TYR:HE1	1.85	0.41
1:B:702:MET:HE2	1:B:702:MET:HB3	1.92	0.41
1:C:34:VAL:HG22	1:C:249:MET:HE1	2.03	0.41
1:C:572:GLN:H	1:C:572:GLN:HG3	1.73	0.41
1:A:186:ALA:HB2	1:A:207:LEU:HA	2.02	0.41
1:C:1007:LYS:HE3	1:C:1007:LYS:HB2	1.82	0.41
1:B:331:ARG:HG2	1:B:370:TYR:HE1	1.86	0.41
1:C:19:THR:O	1:C:19:THR:OG1	2.35	0.41
1:C:228:LEU:HD12	1:C:228:LEU:HA	1.92	0.41
1:C:756:ILE:H	1:C:756:ILE:HG13	1.57	0.41
1:A:1062:THR:OG1	1:A:1063:HIS:ND1	2.52	0.41
6:A:1301:BLA:HA	6:A:1301:BLA:HB	1.68	0.41
1:B:380:GLU:OE1	1:B:460:TYR:OH	2.31	0.41
1:A:946:LEU:HB3	1:A:950:GLU:HG3	2.02	0.40
1:A:1088:CYS:HB2	1:A:1094:ILE:HD13	2.04	0.40
1:A:332:ILE:HB	1:A:369:VAL:HB	2.03	0.40
1:B:75:SER:HA	1:B:76:PRO:HD3	1.96	0.40
1:B:30:ARG:H	1:B:30:ARG:HG3	1.77	0.40
1:B:229:ARG:HG3	1:B:235:LEU:HD21	2.03	0.40
1:C:132:PHE:HE1	1:C:225:LEU:HD13	1.86	0.40
1:C:748:LYS:HD2	1:C:748:LYS:HA	1.79	0.40
1:C:754:PRO:HG2	1:C:759:PHE:HZ	1.87	0.40
1:C:848:TRP:HZ3	1:C:863:GLN:HB2	1.85	0.40
1:A:493:LYS:HE2	1:A:493:LYS:HB3	1.97	0.40
1:A:875:GLN:H	1:A:875:GLN:HG2	1.59	0.40
1:B:776:LYS:HD3	1:B:776:LYS:HA	1.80	0.40
1:A:117:VAL:HG22	1:A:152:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:GLN:HA	1:A:613:GLY:HA3	2.03	0.40
1:B:270:LEU:HB2	1:B:573:VAL:HG11	2.03	0.40
1:C:840:ILE:H	1:C:840:ILE:HG13	1.77	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	1053/1254 (84%)	1006 (96%)	47 (4%)	0	100	100
1	B	1053/1254 (84%)	1025 (97%)	28 (3%)	0	100	100
1	C	1053/1254 (84%)	999 (95%)	54 (5%)	0	100	100
All	All	3159/3762 (84%)	3030 (96%)	129 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	923/1085 (85%)	900 (98%)	23 (2%)	42	43
1	B	923/1085 (85%)	910 (99%)	13 (1%)	62	67
1	C	923/1085 (85%)	904 (98%)	19 (2%)	48	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2769/3255 (85%)	2714 (98%)	55 (2%)	50 53

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	THR
1	A	75	SER
1	A	116	HIS
1	A	117	VAL
1	A	122	CYS
1	A	197	THR
1	A	286	ILE
1	A	376	VAL
1	A	419	THR
1	A	449	VAL
1	A	494	GLN
1	A	526	SER
1	A	605	THR
1	A	651	ASN
1	A	700	CYS
1	A	710	GLU
1	A	717	GLN
1	A	742	GLU
1	A	756	ILE
1	A	790	LEU
1	A	878	LEU
1	A	949	VAL
1	A	1076	ILE
1	B	67	ASN
1	B	75	SER
1	B	81	VAL
1	B	87	ASP
1	B	188	THR
1	B	289	THR
1	B	448	GLN
1	B	449	VAL
1	B	651	ASN
1	B	756	ILE
1	B	796	VAL
1	B	878	LEU
1	B	972	GLN
1	C	29	SER

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Mol	Chain	Res	Type
1	C	59	ASN
1	C	194	ILE
1	C	197	THR
1	C	225	LEU
1	C	235	LEU
1	C	250	MET
1	C	263	ILE
1	C	315	VAL
1	C	376	VAL
1	C	382	ARG
1	C	481	GLU
1	C	605	THR
1	C	756	ILE
1	C	796	VAL
1	C	863	GLN
1	C	895	LYS
1	C	900	LEU
1	C	901	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	422	ASN
1	A	424	ASN
1	A	484	ASN
1	A	620	HIS
1	A	741	GLN
1	A	818	ASN
1	A	875	GLN
1	A	967	GLN
1	A	1020	HIS
1	A	1097	ASN
1	B	17	ASN
1	B	24	HIS
1	B	106	GLN
1	B	116	HIS
1	B	221	ASN
1	B	232	ASN
1	B	288	GLN
1	B	484	ASN
1	B	620	HIS

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Mol	Chain	Res	Type
1	B	749	GLN
1	B	818	ASN
1	B	875	GLN
1	B	931	ASN
1	B	1045	HIS
1	B	1050	HIS
1	B	1096	ASN
1	C	221	ASN
1	C	529	GLN
1	C	572	GLN
1	C	620	HIS
1	C	766	GLN
1	C	815	GLN
1	C	1045	HIS
1	C	1097	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 ⓘ

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	1,2	14,14,15	0.73	0	17,19,21	0.89	0
2	NAG	D	2	2	14,14,15	0.71	0	17,19,21	0.85	0
2	NAG	E	1	1,2	14,14,15	0.38	0	17,19,21	1.61	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	2	2	14,14,15	0.40	0	17,19,21	0.41	0
2	NAG	F	1	1,2	14,14,15	0.70	0	17,19,21	0.90	1 (5%)
2	NAG	F	2	2	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
3	NAG	G	2	3	14,14,15	0.76	0	17,19,21	1.18	2 (11%)
3	BMA	G	3	3	11,11,12	0.87	0	15,15,17	2.42	6 (40%)
3	MAN	G	4	3	11,11,12	0.67	0	15,15,17	1.40	1 (6%)
3	MAN	G	5	3	11,11,12	0.74	0	15,15,17	1.16	1 (6%)
2	NAG	H	1	1,2	14,14,15	0.72	0	17,19,21	1.15	1 (5%)
2	NAG	H	2	2	14,14,15	0.70	0	17,19,21	0.85	0
2	NAG	I	1	1,2	14,14,15	0.69	0	17,19,21	0.93	0
2	NAG	I	2	2	14,14,15	0.71	0	17,19,21	0.84	0
2	NAG	J	1	1,2	14,14,15	0.77	0	17,19,21	1.62	4 (23%)
2	NAG	J	2	2	14,14,15	0.74	0	17,19,21	0.96	1 (5%)
4	NAG	K	1	4,1	14,14,15	0.84	0	17,19,21	2.01	6 (35%)
4	NAG	K	2	4	14,14,15	0.74	0	17,19,21	1.35	2 (11%)
4	BMA	K	3	4	11,11,12	0.86	0	15,15,17	2.44	4 (26%)
4	MAN	K	4	4	11,11,12	0.79	0	15,15,17	1.23	2 (13%)
4	MAN	K	5	4	11,11,12	0.83	0	15,15,17	1.08	1 (6%)
2	NAG	L	1	1,2	14,14,15	0.73	0	17,19,21	1.10	1 (5%)
2	NAG	L	2	2	14,14,15	0.70	0	17,19,21	1.04	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.74	0	17,19,21	1.12	1 (5%)
2	NAG	M	2	2	14,14,15	0.71	0	17,19,21	0.85	0
2	NAG	N	1	1,2	14,14,15	0.80	0	17,19,21	1.88	3 (17%)
2	NAG	N	2	2	14,14,15	0.73	0	17,19,21	1.12	2 (11%)
2	NAG	O	1	1,2	14,14,15	0.77	0	17,19,21	1.78	4 (23%)
2	NAG	O	2	2	14,14,15	0.70	0	17,19,21	1.10	1 (5%)
5	NAG	P	1	1,5	14,14,15	0.73	0	17,19,21	1.09	2 (11%)
5	NAG	P	2	5	14,14,15	0.76	0	17,19,21	1.18	2 (11%)
5	BMA	P	3	5	11,11,12	0.88	0	15,15,17	2.40	5 (33%)
5	MAN	P	4	5	11,11,12	0.70	0	15,15,17	1.28	1 (6%)
2	NAG	Q	1	1,2	14,14,15	0.69	0	17,19,21	0.92	1 (5%)
2	NAG	Q	2	2	14,14,15	0.72	0	17,19,21	1.46	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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
3	MAN	G	5	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	BMA	K	3	4	-	1/2/19/22	0/1/1/1
4	MAN	K	4	4	-	2/2/19/22	0/1/1/1
4	MAN	K	5	4	-	0/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	1/6/23/26	0/1/1/1
5	BMA	P	3	5	-	0/2/19/22	0/1/1/1
5	MAN	P	4	5	-	0/2/19/22	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	3	BMA	C1-O5-C5	7.42	122.25	112.19
5	P	3	BMA	C1-O5-C5	7.07	121.77	112.19
3	G	3	BMA	C1-O5-C5	7.04	121.74	112.19
2	E	1	NAG	C2-N2-C7	6.24	131.79	122.90
4	K	1	NAG	O5-C1-C2	-5.13	103.18	111.29
2	O	1	NAG	C2-N2-C7	4.83	129.78	122.90
2	N	1	NAG	C2-N2-C7	4.50	129.30	122.90
3	G	4	MAN	C1-O5-C5	4.25	117.95	112.19
2	Q	2	NAG	C2-N2-C7	4.24	128.94	122.90
5	P	4	MAN	C1-O5-C5	3.93	117.52	112.19
2	J	1	NAG	C4-C3-C2	3.61	116.31	111.02
2	N	1	NAG	O5-C1-C2	-3.40	105.92	111.29
3	G	5	MAN	C1-O5-C5	3.36	116.74	112.19
3	G	3	BMA	C3-C4-C5	3.02	115.63	110.24
2	J	1	NAG	C2-N2-C7	3.02	127.20	122.90
5	P	2	NAG	C1-O5-C5	2.99	116.25	112.19
2	O	2	NAG	C2-N2-C7	2.98	127.15	122.90
4	K	1	NAG	O4-C4-C3	-2.98	103.47	110.35
4	K	1	NAG	C3-C4-C5	2.97	115.55	110.24
4	K	2	NAG	C4-C3-C2	2.97	115.37	111.02
4	K	1	NAG	C1-C2-N2	2.95	115.53	110.49
4	K	3	BMA	C2-C3-C4	2.95	116.00	110.89
4	K	4	MAN	C1-O5-C5	2.91	116.13	112.19
2	L	1	NAG	C2-N2-C7	2.90	127.03	122.90
3	G	2	NAG	C1-O5-C5	2.85	116.05	112.19
5	P	3	BMA	C3-C4-C5	2.81	115.25	110.24
4	K	2	NAG	C2-N2-C7	2.77	126.85	122.90
5	P	1	NAG	C1-O5-C5	2.76	115.94	112.19
2	J	1	NAG	O4-C4-C3	-2.75	104.00	110.35
2	L	2	NAG	C2-N2-C7	2.73	126.80	122.90
2	N	2	NAG	C2-N2-C7	2.67	126.71	122.90
2	M	1	NAG	C2-N2-C7	2.65	126.67	122.90
5	P	3	BMA	C2-C3-C4	2.62	115.43	110.89
2	H	1	NAG	C2-N2-C7	2.60	126.60	122.90
3	G	3	BMA	C2-C3-C4	2.51	115.24	110.89
3	G	2	NAG	O4-C4-C3	-2.50	104.58	110.35
2	J	1	NAG	O5-C1-C2	-2.43	107.44	111.29
3	G	3	BMA	O3-C3-C2	-2.31	105.57	109.99
2	N	1	NAG	O4-C4-C3	-2.31	105.01	110.35
5	P	2	NAG	O4-C4-C3	-2.30	105.03	110.35
5	P	3	BMA	O3-C3-C2	-2.26	105.66	109.99
4	K	1	NAG	C4-C3-C2	2.25	114.31	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	BMA	O4-C4-C3	-2.25	105.15	110.35
4	K	3	BMA	O3-C3-C2	-2.24	105.71	109.99
2	O	1	NAG	O5-C1-C2	-2.23	107.77	111.29
4	K	3	BMA	C3-C4-C5	2.21	114.18	110.24
2	N	2	NAG	C1-O5-C5	2.19	115.17	112.19
2	F	2	NAG	C1-O5-C5	2.19	115.17	112.19
4	K	5	MAN	C1-O5-C5	2.19	115.16	112.19
2	O	1	NAG	C1-O5-C5	2.13	115.07	112.19
4	K	1	NAG	O5-C5-C4	2.13	116.00	110.83
2	J	2	NAG	C1-O5-C5	2.12	115.07	112.19
5	P	3	BMA	O4-C4-C3	-2.12	105.45	110.35
2	O	1	NAG	O7-C7-N2	2.12	125.85	121.95
2	Q	1	NAG	O5-C1-C2	-2.10	107.98	111.29
5	P	1	NAG	O3-C3-C2	-2.08	105.17	109.47
4	K	4	MAN	C1-C2-C3	2.06	112.20	109.67
2	Q	2	NAG	O7-C7-N2	2.04	125.71	121.95
3	G	1	NAG	C1-O5-C5	2.04	114.95	112.19
3	G	3	BMA	O5-C5-C4	2.02	115.75	110.83
2	F	1	NAG	O5-C1-C2	-2.02	108.10	111.29

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	4	MAN	O5-C5-C6-O6
4	K	4	MAN	C4-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	N	2	NAG	C8-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2

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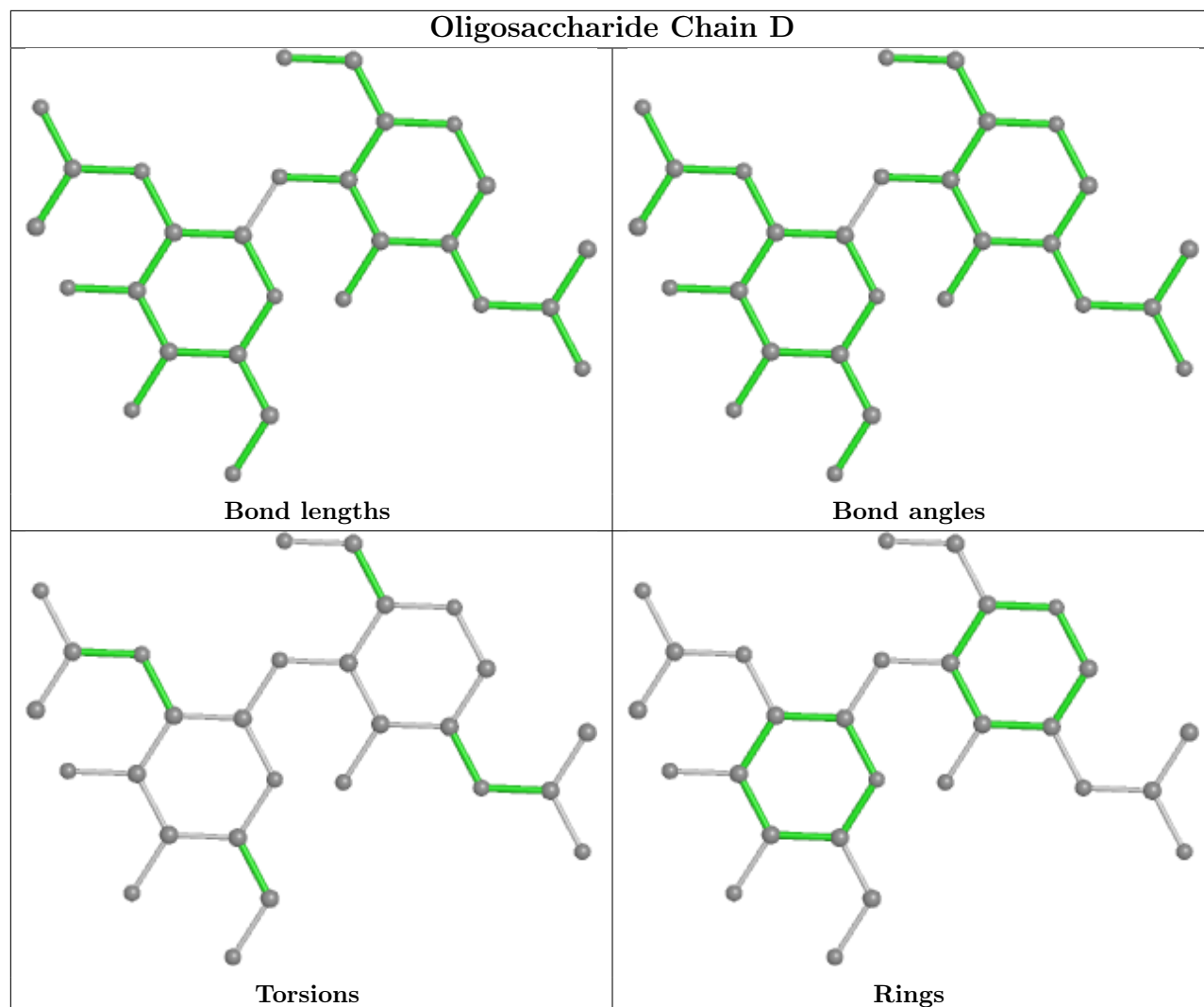
Mol	Chain	Res	Type	Atoms
2	O	2	NAG	C8-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2
5	P	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C1-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7
2	N	1	NAG	C3-C2-N2-C7
2	O	1	NAG	C1-C2-N2-C7
4	K	1	NAG	O5-C5-C6-O6
2	O	1	NAG	C3-C2-N2-C7
2	Q	2	NAG	C3-C2-N2-C7

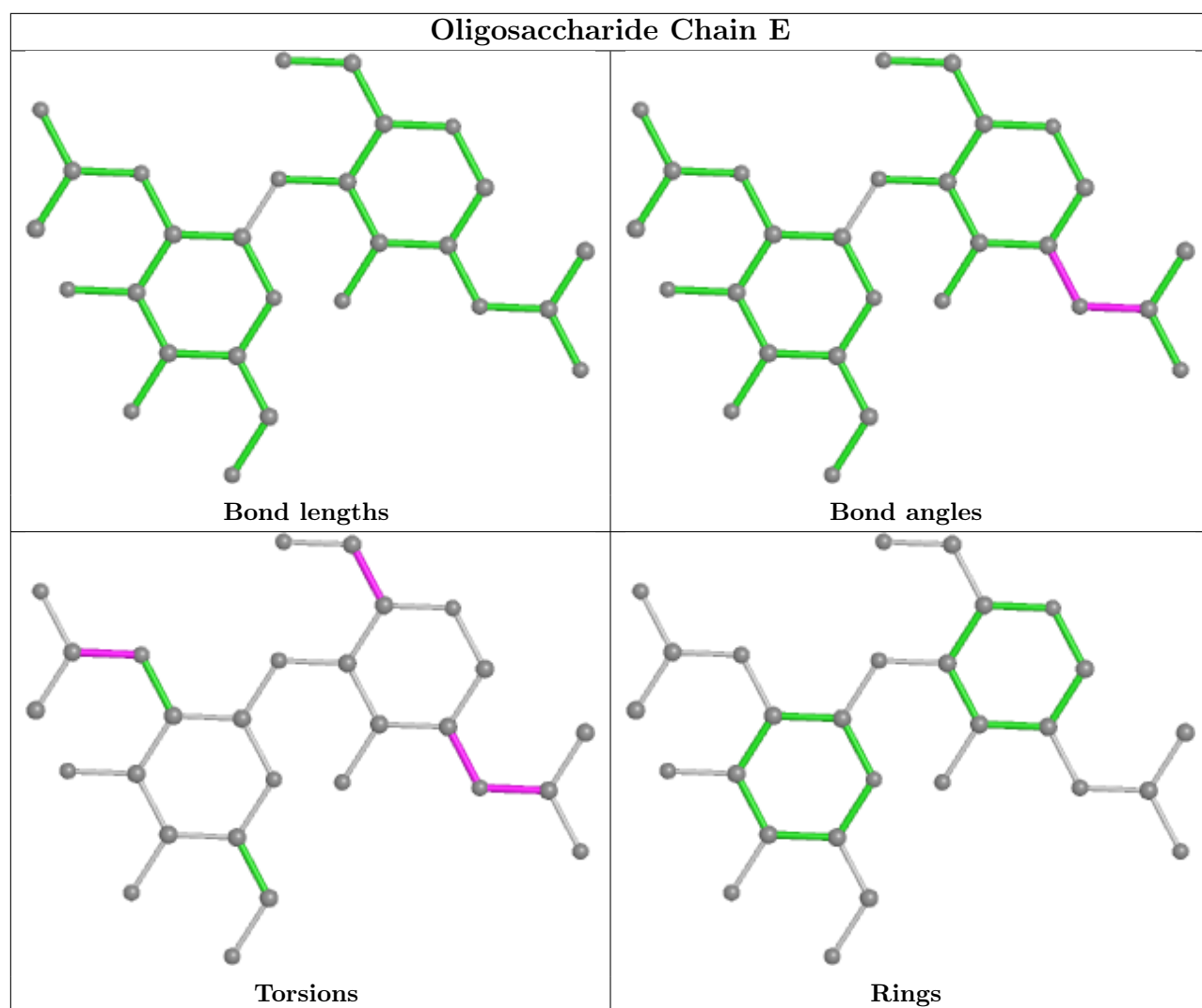
There are no ring outliers.

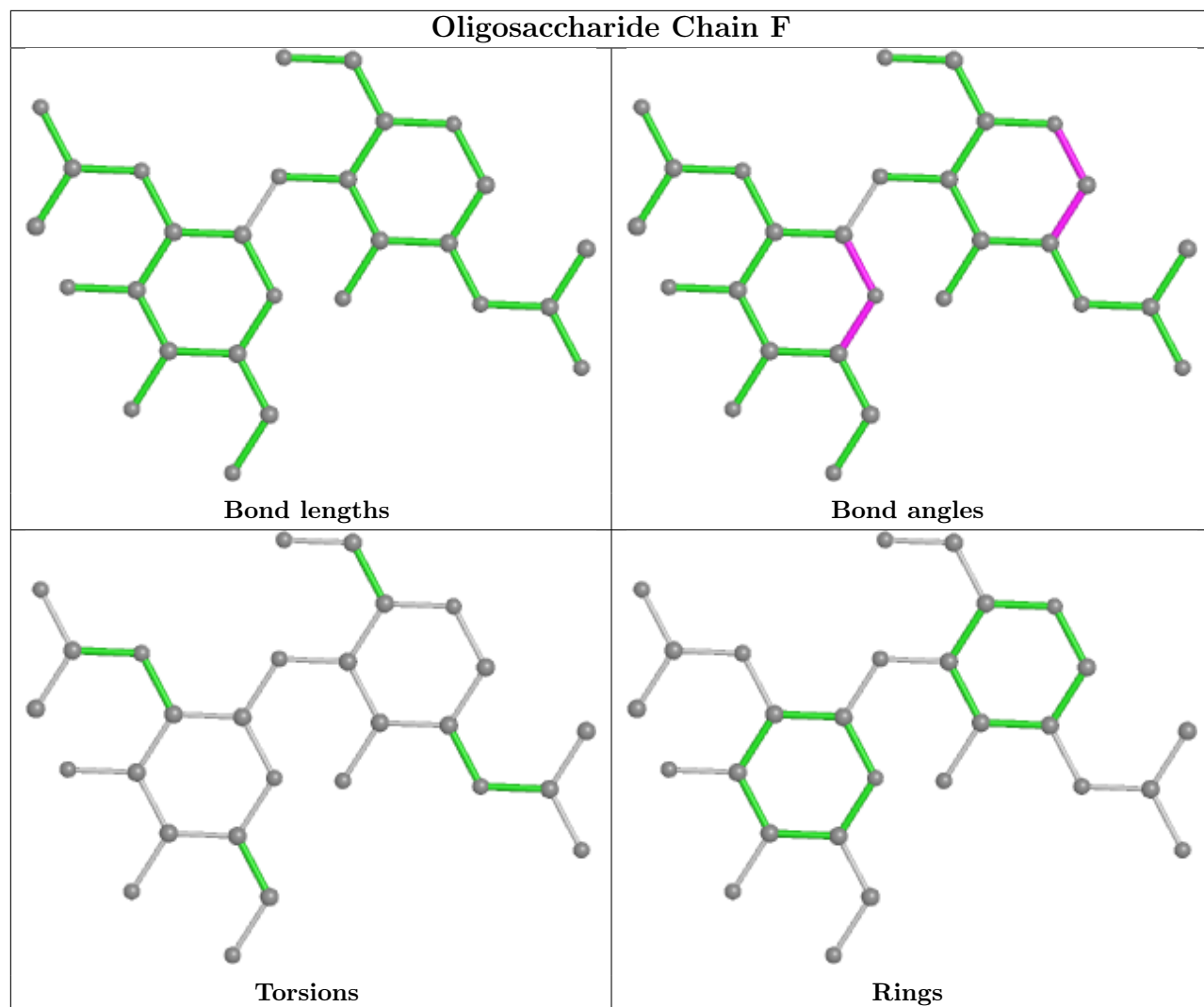
5 monomers are involved in 5 short contacts:

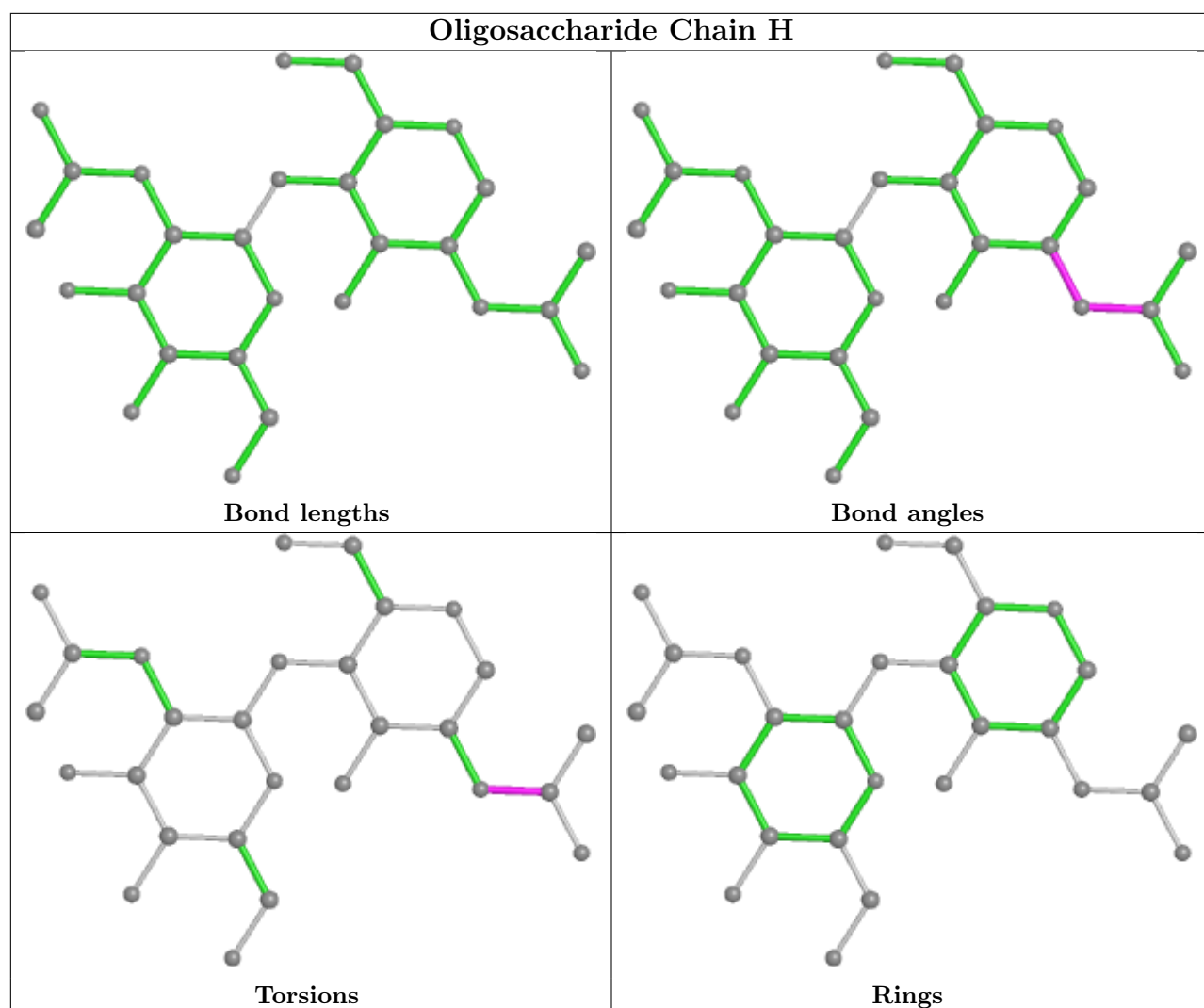
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	1	0
2	E	1	NAG	1	0
2	N	2	NAG	1	0
2	J	1	NAG	1	0
3	G	1	NAG	1	0

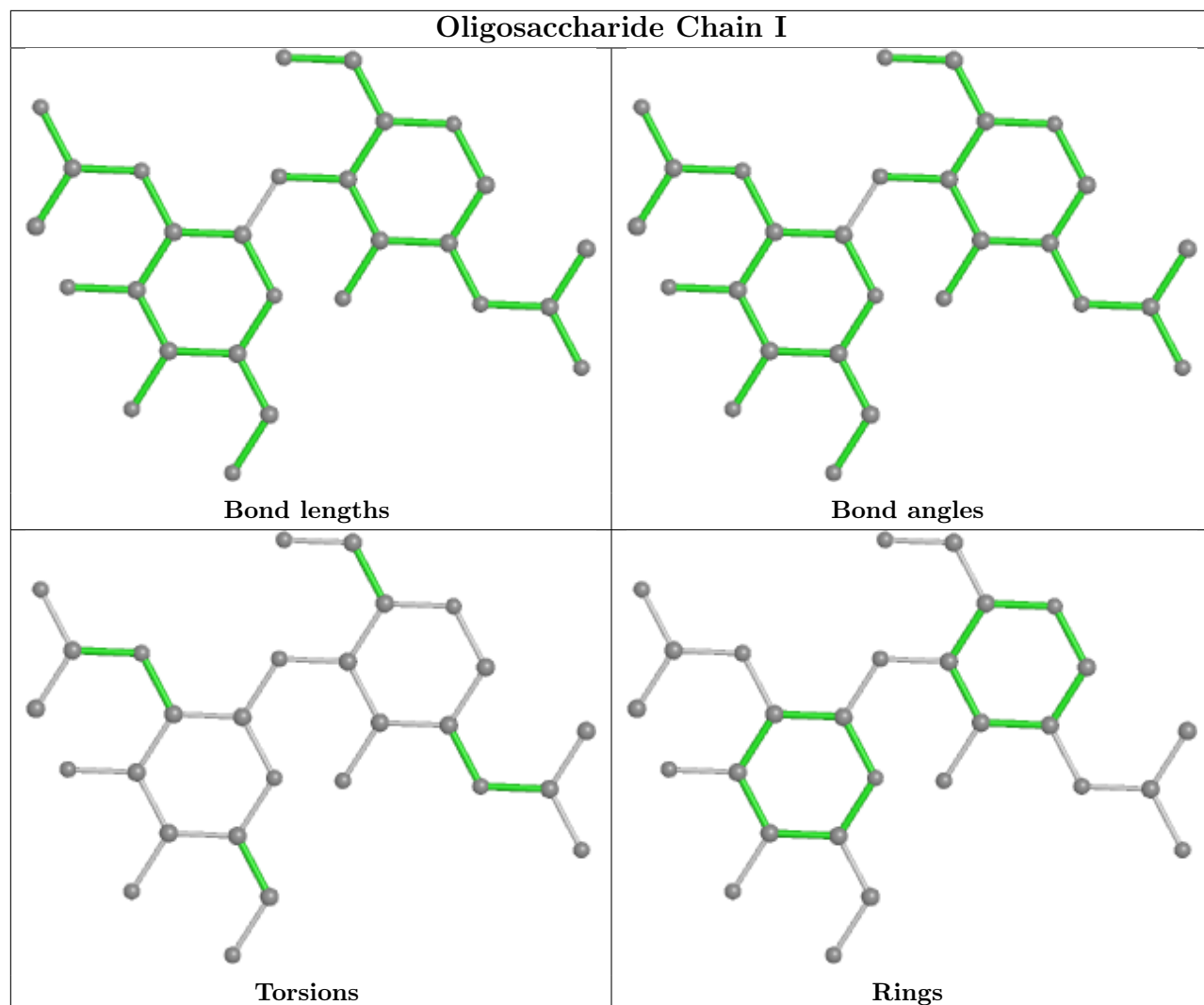
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

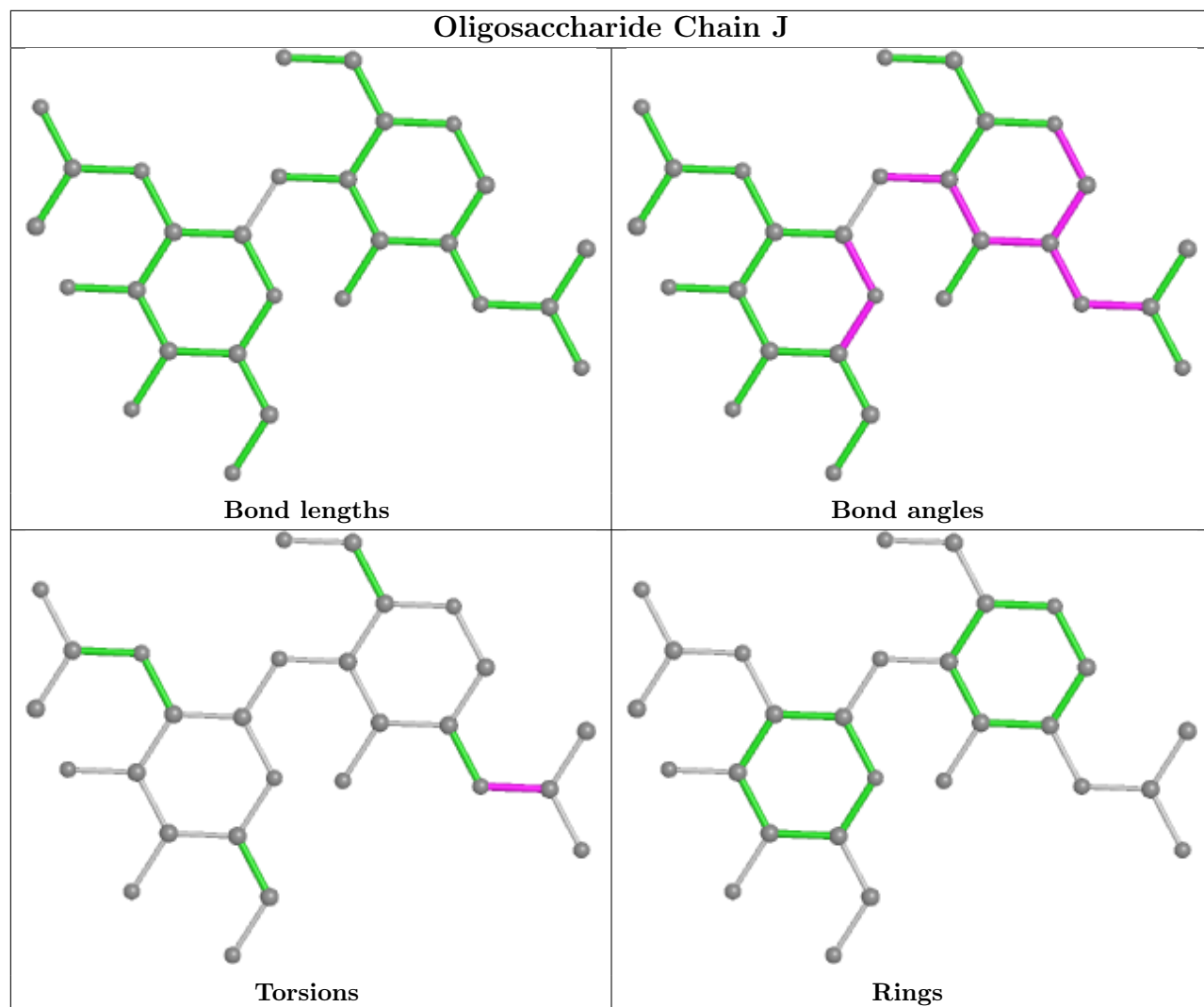


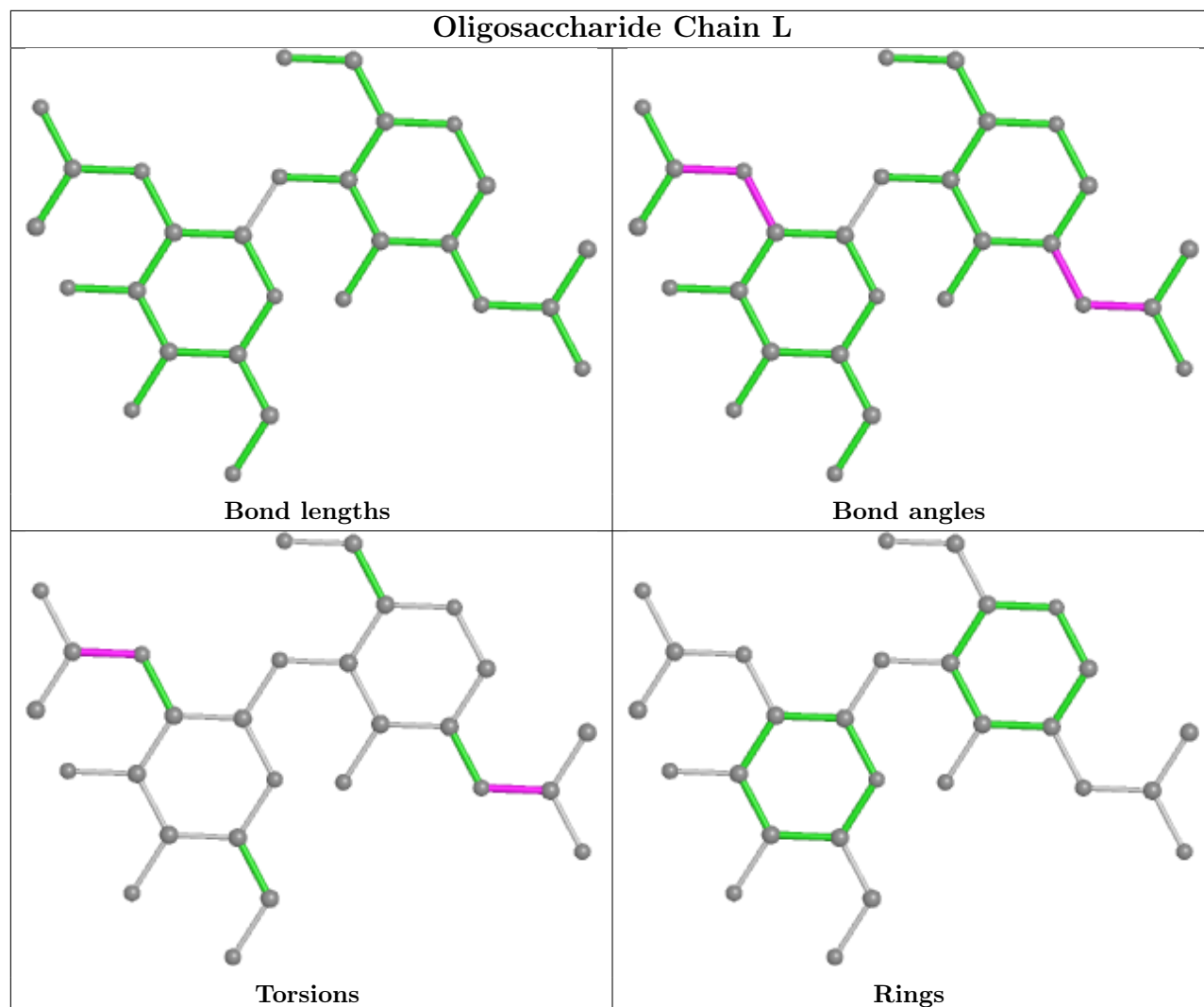


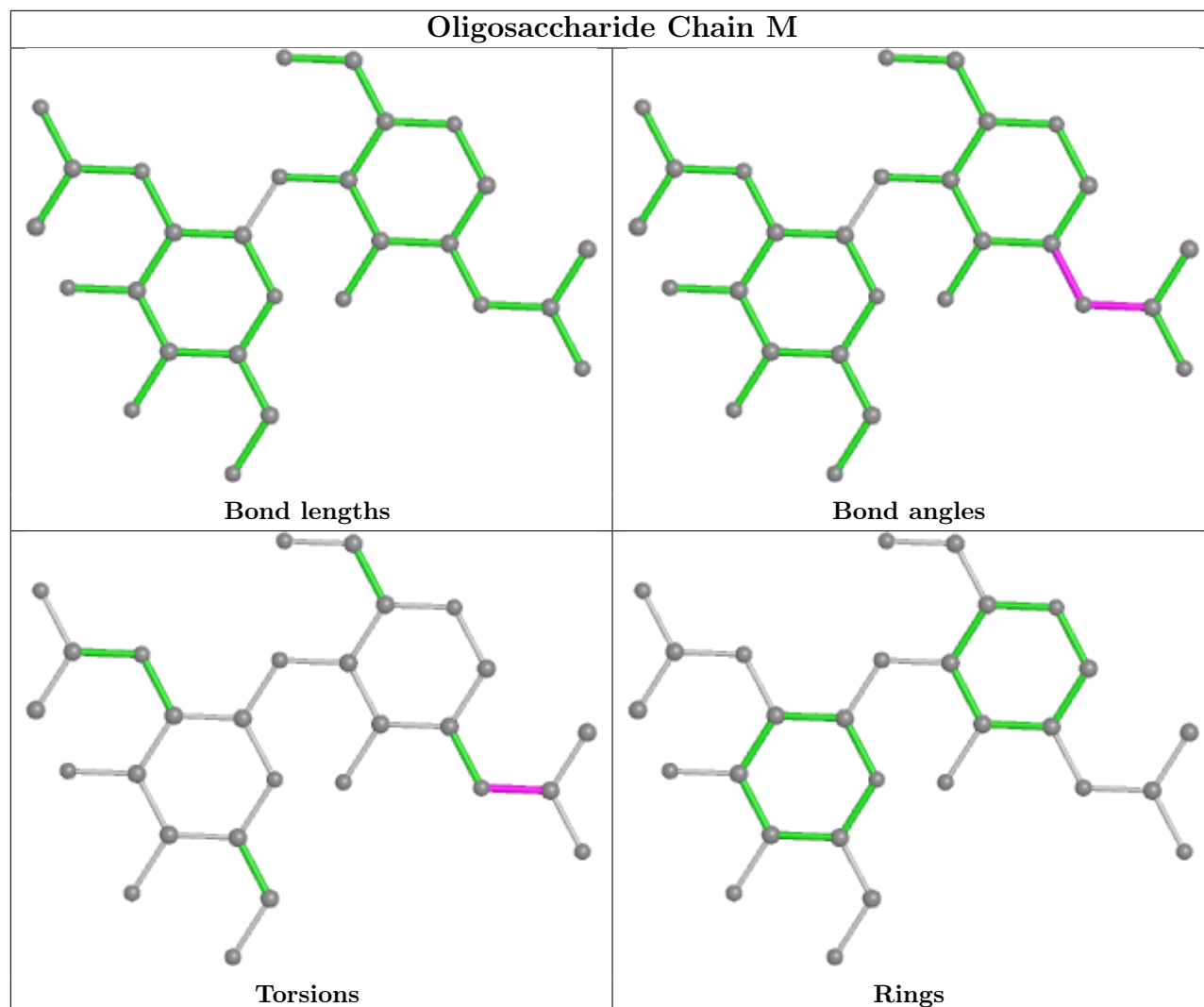


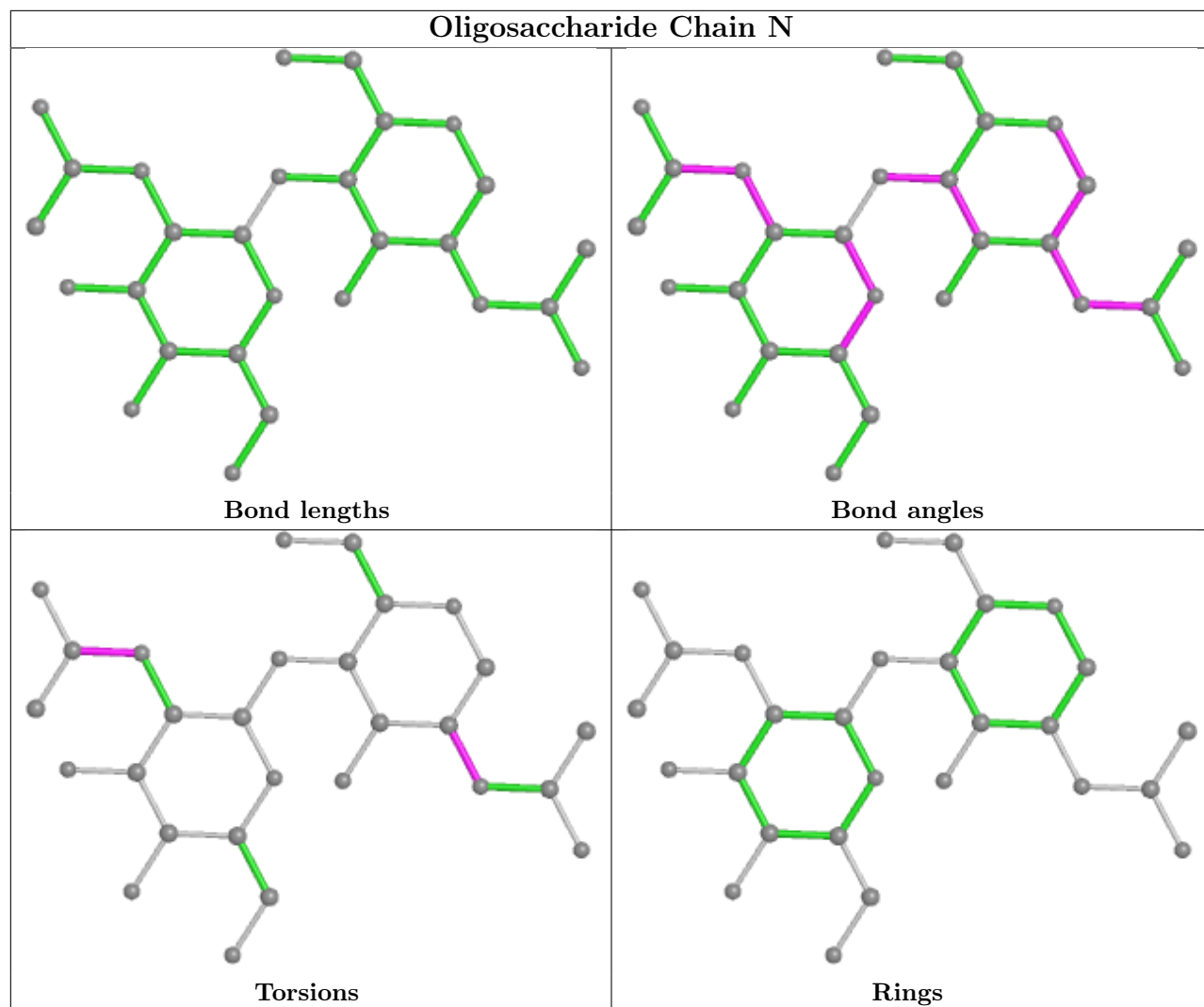


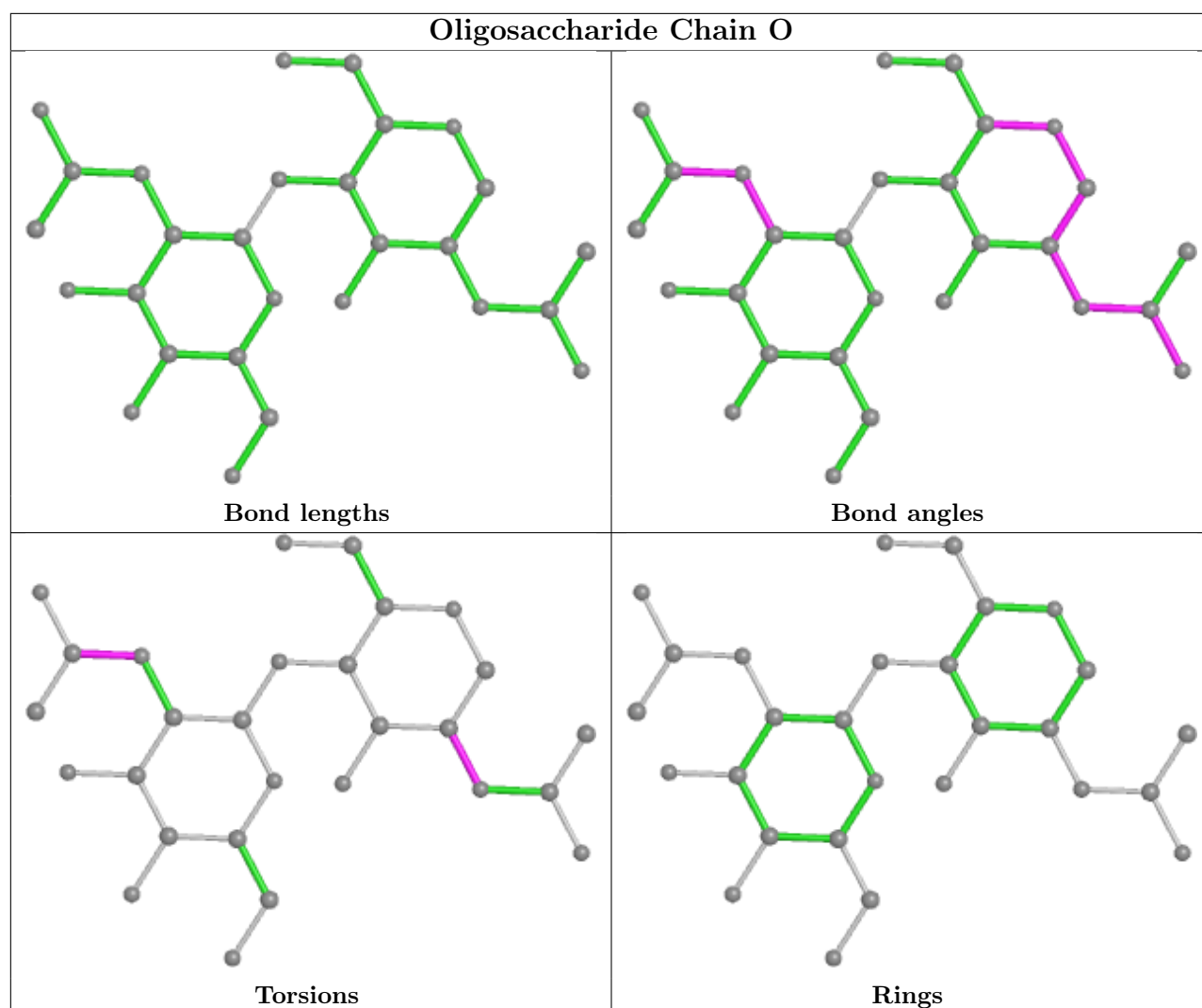


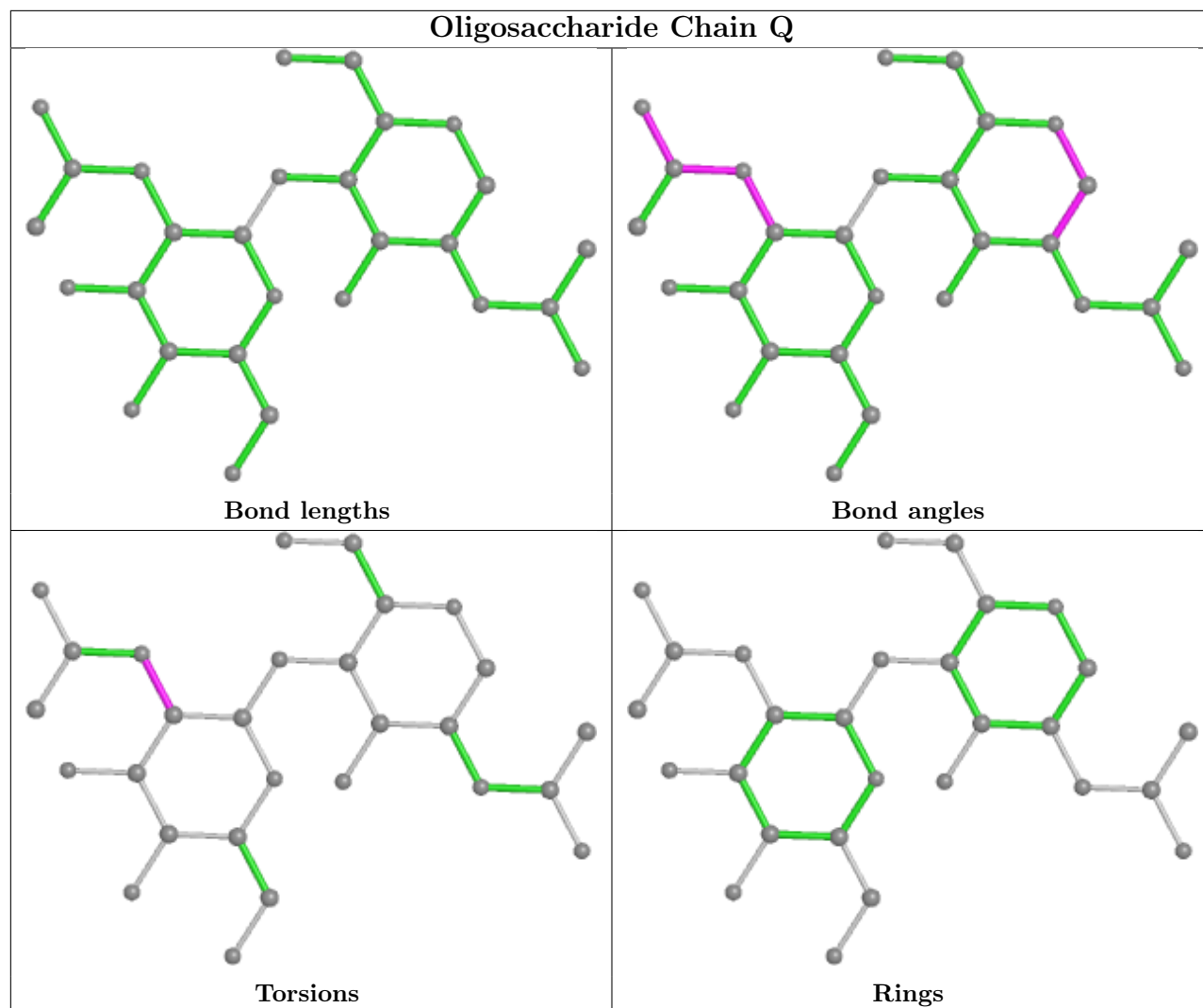


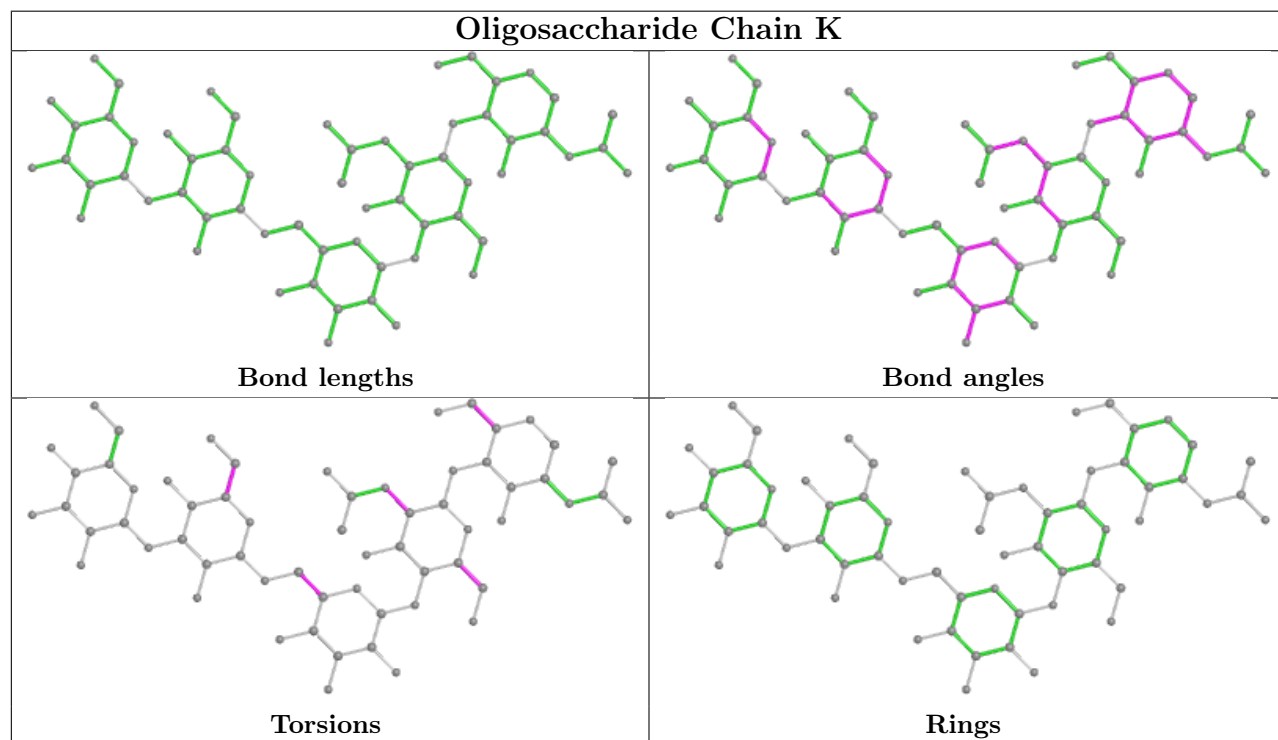
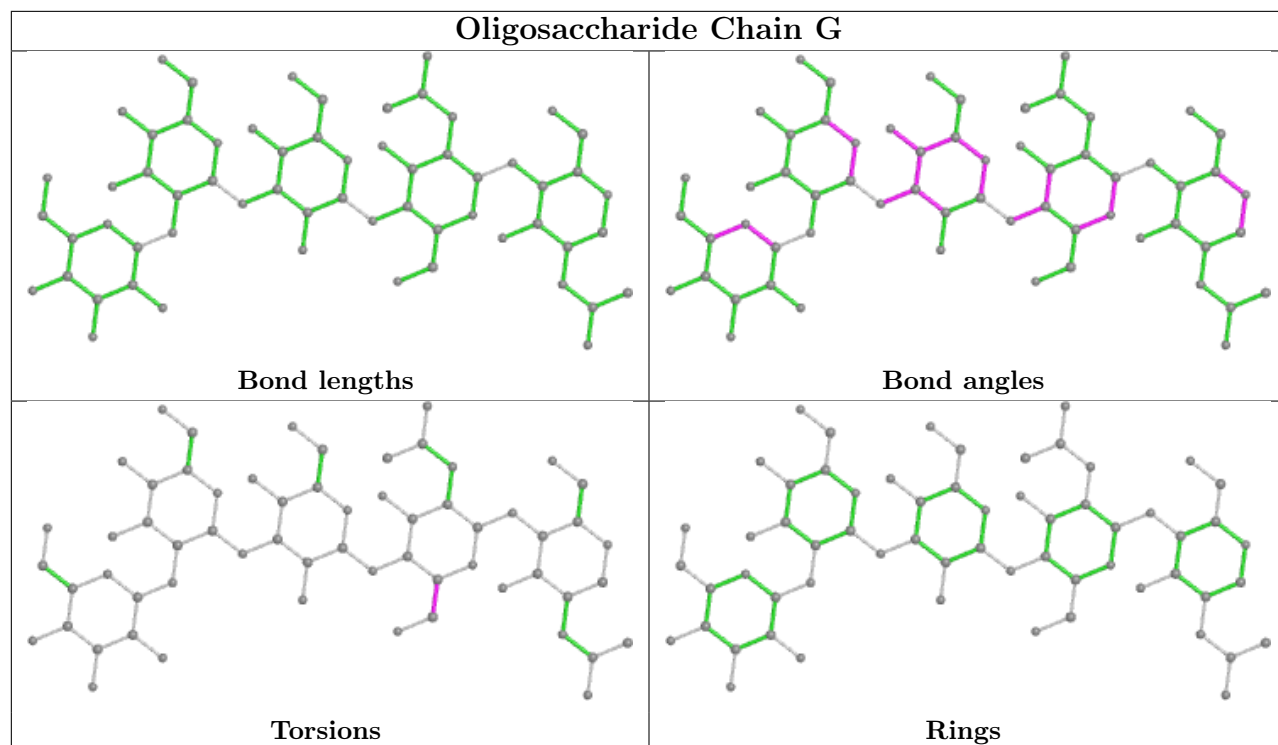


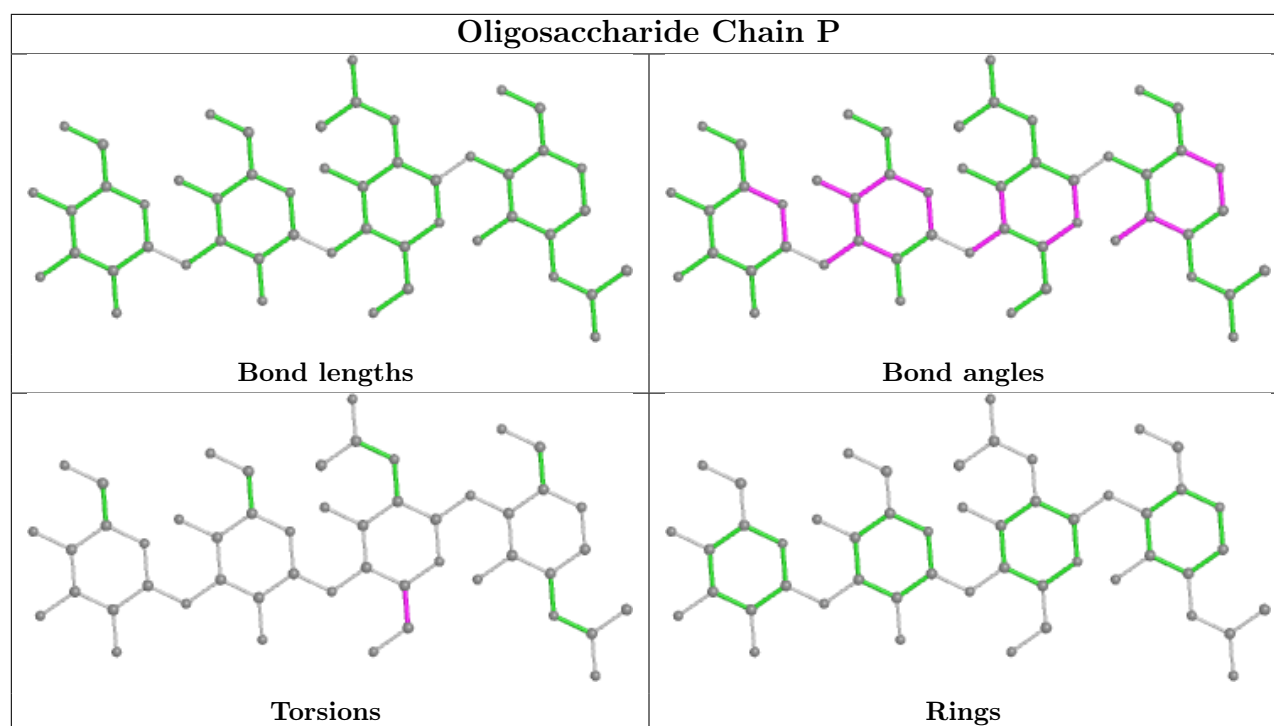












5.6 Ligand geometry [i](#)

40 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	$\# Z > 2$
7	NAG	A	1307	1	14,14,15	0.73	0	17,19,21	1.15	2 (11%)
6	BLA	B	1302	-	42,46,46	1.28	5 (11%)	53,67,67	1.10	4 (7%)
7	NAG	A	1310	1	14,14,15	0.69	0	17,19,21	1.56	2 (11%)
7	NAG	B	1310	1	14,14,15	0.71	0	17,19,21	1.03	1 (5%)
7	NAG	B	1309	1	14,14,15	0.74	0	17,19,21	0.99	1 (5%)
7	NAG	C	1312	1	14,14,15	0.71	0	17,19,21	0.86	0
7	NAG	C	1311	1	14,14,15	0.72	0	17,19,21	0.90	1 (5%)
7	NAG	A	1304	1	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
7	NAG	C	1313	1	14,14,15	0.72	0	17,19,21	1.14	2 (11%)
7	NAG	B	1308	1	14,14,15	0.72	0	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	1306	1	14,14,15	0.69	0	17,19,21	0.87	0
7	NAG	A	1303	1	14,14,15	0.72	0	17,19,21	0.88	0
7	NAG	B	1311	1	14,14,15	0.70	0	17,19,21	0.86	0
7	NAG	A	1306	1	14,14,15	0.71	0	17,19,21	1.01	1 (5%)
7	NAG	B	1313	1	14,14,15	0.73	0	17,19,21	1.45	2 (11%)
7	NAG	C	1307	1	14,14,15	0.74	0	17,19,21	1.13	1 (5%)
7	NAG	C	1310	1	14,14,15	0.73	0	17,19,21	1.03	1 (5%)
7	NAG	A	1309	1	14,14,15	0.69	0	17,19,21	1.03	1 (5%)
7	NAG	A	1308	1	14,14,15	0.71	0	17,19,21	0.88	0
7	NAG	B	1304	1	14,14,15	0.71	0	17,19,21	0.88	0
7	NAG	C	1304	1	14,14,15	0.71	0	17,19,21	1.08	1 (5%)
7	NAG	A	1312	1	14,14,15	0.69	0	17,19,21	1.04	2 (11%)
7	NAG	C	1308	1	14,14,15	0.72	0	17,19,21	0.90	0
8	EIC	B	1301	-	19,19,19	1.31	2 (10%)	19,19,19	0.94	0
8	EIC	A	1313	-	19,19,19	1.31	2 (10%)	19,19,19	0.94	0
8	EIC	C	1301	-	19,19,19	1.31	2 (10%)	19,19,19	0.94	0
7	NAG	A	1305	1	14,14,15	0.71	0	17,19,21	1.07	1 (5%)
7	NAG	B	1305	1	14,14,15	0.73	0	17,19,21	0.97	1 (5%)
7	NAG	B	1306	1	14,14,15	0.71	0	17,19,21	1.48	2 (11%)
7	NAG	B	1303	1	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
7	NAG	C	1305	1	14,14,15	0.71	0	17,19,21	1.08	2 (11%)
7	NAG	C	1314	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
7	NAG	A	1302	1	14,14,15	0.70	0	17,19,21	1.49	3 (17%)
7	NAG	C	1303	1	14,14,15	0.74	0	17,19,21	0.93	1 (5%)
7	NAG	A	1311	1	14,14,15	0.69	0	17,19,21	0.92	1 (5%)
7	NAG	B	1307	1	14,14,15	0.75	0	17,19,21	0.99	1 (5%)
6	BLA	A	1301	-	42,46,46	1.27	5 (11%)	53,67,67	1.11	4 (7%)
6	BLA	C	1302	-	42,46,46	1.28	5 (11%)	53,67,67	1.11	4 (7%)
7	NAG	B	1312	1	14,14,15	0.72	0	17,19,21	1.00	1 (5%)
7	NAG	C	1309	1	14,14,15	0.72	0	17,19,21	1.44	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
7	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
6	BLA	B	1302	-	-	6/26/74/74	0/4/4/4
7	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1313	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
8	EIC	B	1301	-	-	6/17/17/17	-
8	EIC	A	1313	-	-	5/17/17/17	-
8	EIC	C	1301	-	-	6/17/17/17	-
7	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1314	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
6	BLA	A	1301	-	-	8/26/74/74	0/4/4/4
6	BLA	C	1302	-	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1312	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1309	1	-	1/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1302	BLA	CHA-C4D	3.94	1.38	1.35
6	B	1302	BLA	CHA-C4D	3.90	1.38	1.35
6	A	1301	BLA	CHA-C4D	3.82	1.38	1.35
8	B	1301	EIC	C13-C12	3.67	1.53	1.31
8	A	1313	EIC	C13-C12	3.67	1.53	1.31
8	C	1301	EIC	C13-C12	3.67	1.53	1.31
8	B	1301	EIC	C10-C9	3.65	1.53	1.31
8	C	1301	EIC	C10-C9	3.65	1.52	1.31
8	A	1313	EIC	C10-C9	3.65	1.52	1.31
6	A	1301	BLA	CAB-C3B	-2.83	1.39	1.47
6	A	1301	BLA	CAC-C3C	-2.81	1.39	1.47
6	B	1302	BLA	CAB-C3B	-2.79	1.39	1.47
6	C	1302	BLA	CAB-C3B	-2.77	1.39	1.47
6	B	1302	BLA	CAC-C3C	-2.77	1.39	1.47
6	C	1302	BLA	CAC-C3C	-2.72	1.40	1.47
6	B	1302	BLA	C3B-C2B	2.42	1.42	1.37
6	A	1301	BLA	C3B-C2B	2.36	1.42	1.37
6	C	1302	BLA	C3B-C2B	2.35	1.42	1.37
6	A	1301	BLA	C3C-C4C	-2.26	1.41	1.45
6	B	1302	BLA	C3C-C4C	-2.21	1.41	1.45
6	C	1302	BLA	C3C-C4C	-2.12	1.42	1.45

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1310	NAG	C2-N2-C7	4.36	129.11	122.90
7	B	1313	NAG	C2-N2-C7	4.35	129.10	122.90
7	C	1309	NAG	C2-N2-C7	4.33	129.07	122.90
7	A	1302	NAG	C2-N2-C7	4.27	128.98	122.90
7	B	1306	NAG	C2-N2-C7	4.26	128.97	122.90
6	C	1302	BLA	CHA-C4D-ND	-3.44	124.05	128.83
6	A	1301	BLA	CHA-C4D-ND	-3.42	124.08	128.83
6	B	1302	BLA	CHA-C4D-ND	-3.41	124.09	128.83
7	C	1307	NAG	C2-N2-C7	2.96	127.12	122.90
7	C	1304	NAG	C2-N2-C7	2.85	126.96	122.90
7	A	1307	NAG	C1-O5-C5	2.83	116.02	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1302	BLA	CMC-C2C-C1C	2.82	128.03	121.39
6	C	1302	BLA	CMC-C2C-C1C	2.80	127.97	121.39
6	A	1301	BLA	CMC-C2C-C1C	2.79	127.96	121.39
7	B	1312	NAG	C1-O5-C5	2.79	115.97	112.19
7	C	1310	NAG	C1-O5-C5	2.77	115.95	112.19
7	A	1310	NAG	C1-O5-C5	2.76	115.93	112.19
7	A	1305	NAG	C2-N2-C7	2.74	126.80	122.90
7	C	1313	NAG	C2-N2-C7	2.74	126.80	122.90
7	A	1309	NAG	C2-N2-C7	2.73	126.80	122.90
7	A	1304	NAG	C2-N2-C7	2.69	126.73	122.90
7	C	1313	NAG	C1-O5-C5	2.67	115.81	112.19
7	B	1309	NAG	C1-O5-C5	2.66	115.79	112.19
7	B	1308	NAG	C2-N2-C7	2.64	126.66	122.90
7	B	1303	NAG	C2-N2-C7	2.61	126.62	122.90
7	A	1312	NAG	C2-N2-C7	2.59	126.59	122.90
7	A	1306	NAG	C2-N2-C7	2.57	126.56	122.90
7	A	1307	NAG	C2-N2-C7	2.54	126.51	122.90
6	A	1301	BLA	CMB-C2B-C1B	2.52	127.32	124.17
7	C	1314	NAG	C2-N2-C7	2.51	126.47	122.90
6	B	1302	BLA	CMB-C2B-C1B	2.50	127.29	124.17
6	C	1302	BLA	C1A-CHA-C4D	-2.50	125.82	128.81
7	B	1305	NAG	C1-O5-C5	2.50	115.57	112.19
7	C	1305	NAG	C2-N2-C7	2.46	126.41	122.90
7	B	1310	NAG	C2-N2-C7	2.46	126.41	122.90
6	B	1302	BLA	C1A-CHA-C4D	-2.41	125.93	128.81
6	C	1302	BLA	CMB-C2B-C1B	2.37	127.12	124.17
7	B	1307	NAG	C2-N2-C7	2.33	126.23	122.90
6	A	1301	BLA	C1A-CHA-C4D	-2.31	126.05	128.81
7	A	1311	NAG	C1-O5-C5	2.19	115.15	112.19
7	A	1302	NAG	C1-O5-C5	2.19	115.15	112.19
7	A	1312	NAG	C1-O5-C5	2.12	115.06	112.19
7	C	1303	NAG	O5-C1-C2	-2.11	107.96	111.29
7	C	1305	NAG	C1-O5-C5	2.08	115.01	112.19
7	C	1311	NAG	C1-O5-C5	2.07	115.00	112.19
7	B	1306	NAG	C1-O5-C5	2.03	114.95	112.19
7	B	1313	NAG	O7-C7-N2	2.02	125.66	121.95
7	C	1309	NAG	O7-C7-N2	2.01	125.65	121.95
7	A	1302	NAG	O7-C7-N2	2.00	125.64	121.95

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1301	BLA	ND-C4D-CHA-C1A
6	A	1301	BLA	C3D-C4D-CHA-C1A
6	B	1302	BLA	ND-C4D-CHA-C1A
6	C	1302	BLA	ND-C4D-CHA-C1A
6	C	1302	BLA	C3D-C4D-CHA-C1A
8	A	1313	EIC	C11-C12-C13-C14
8	C	1301	EIC	C11-C12-C13-C14
8	B	1301	EIC	C11-C12-C13-C14
7	A	1304	NAG	C8-C7-N2-C2
7	A	1304	NAG	O7-C7-N2-C2
7	A	1305	NAG	C8-C7-N2-C2
7	A	1305	NAG	O7-C7-N2-C2
7	A	1306	NAG	C8-C7-N2-C2
7	A	1306	NAG	O7-C7-N2-C2
7	A	1307	NAG	C8-C7-N2-C2
7	A	1307	NAG	O7-C7-N2-C2
7	A	1309	NAG	C8-C7-N2-C2
7	A	1309	NAG	O7-C7-N2-C2
7	A	1312	NAG	C8-C7-N2-C2
7	A	1312	NAG	O7-C7-N2-C2
7	B	1303	NAG	C8-C7-N2-C2
7	B	1303	NAG	O7-C7-N2-C2
7	B	1308	NAG	C8-C7-N2-C2
7	B	1308	NAG	O7-C7-N2-C2
7	B	1310	NAG	C8-C7-N2-C2
7	B	1310	NAG	O7-C7-N2-C2
7	C	1304	NAG	C8-C7-N2-C2
7	C	1304	NAG	O7-C7-N2-C2
7	C	1305	NAG	C8-C7-N2-C2
7	C	1305	NAG	O7-C7-N2-C2
7	C	1307	NAG	C8-C7-N2-C2
7	C	1307	NAG	O7-C7-N2-C2
7	C	1313	NAG	C8-C7-N2-C2
7	C	1313	NAG	O7-C7-N2-C2
7	C	1314	NAG	C8-C7-N2-C2
7	C	1314	NAG	O7-C7-N2-C2
8	A	1313	EIC	C1-C2-C3-C4
8	B	1301	EIC	C1-C2-C3-C4
8	C	1301	EIC	C1-C2-C3-C4
7	C	1310	NAG	O5-C5-C6-O6
8	B	1301	EIC	C5-C6-C7-C8
6	A	1301	BLA	C2C-C3C-CAC-CBC
6	B	1302	BLA	C3D-C4D-CHA-C1A

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Mol	Chain	Res	Type	Atoms
8	A	1313	EIC	C12-C13-C14-C15
7	A	1304	NAG	O5-C5-C6-O6
8	C	1301	EIC	C12-C13-C14-C15
7	B	1312	NAG	O5-C5-C6-O6
7	A	1302	NAG	O5-C5-C6-O6
7	C	1303	NAG	O5-C5-C6-O6
7	C	1314	NAG	O5-C5-C6-O6
8	B	1301	EIC	C9-C10-C11-C12
8	C	1301	EIC	C5-C6-C7-C8
6	B	1302	BLA	C2C-C3C-CAC-CBC
6	C	1302	BLA	C2C-C3C-CAC-CBC
6	A	1301	BLA	C4C-C3C-CAC-CBC
7	C	1310	NAG	C4-C5-C6-O6
7	A	1302	NAG	C3-C2-N2-C7
7	B	1306	NAG	C3-C2-N2-C7
7	B	1313	NAG	C3-C2-N2-C7
6	B	1302	BLA	C4C-C3C-CAC-CBC
6	C	1302	BLA	C4C-C3C-CAC-CBC
6	C	1302	BLA	CAA-CBA-CGA-O2A
8	C	1301	EIC	O2-C1-C2-C3
6	C	1302	BLA	CAA-CBA-CGA-O1A
6	C	1302	BLA	CAD-CBD-CGD-O2D
6	A	1301	BLA	CAD-CBD-CGD-O2D
8	A	1313	EIC	O2-C1-C2-C3
8	B	1301	EIC	O2-C1-C2-C3
8	C	1301	EIC	O1-C1-C2-C3
6	A	1301	BLA	CAA-CBA-CGA-O2A
6	B	1302	BLA	CAD-CBD-CGD-O2D
6	A	1301	BLA	CAA-CBA-CGA-O1A
8	A	1313	EIC	O1-C1-C2-C3
8	B	1301	EIC	O1-C1-C2-C3
6	B	1302	BLA	CAD-CBD-CGD-O1D
6	A	1301	BLA	CAD-CBD-CGD-O1D
6	C	1302	BLA	CAD-CBD-CGD-O1D
7	A	1310	NAG	C3-C2-N2-C7
7	C	1309	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 8 short contacts:

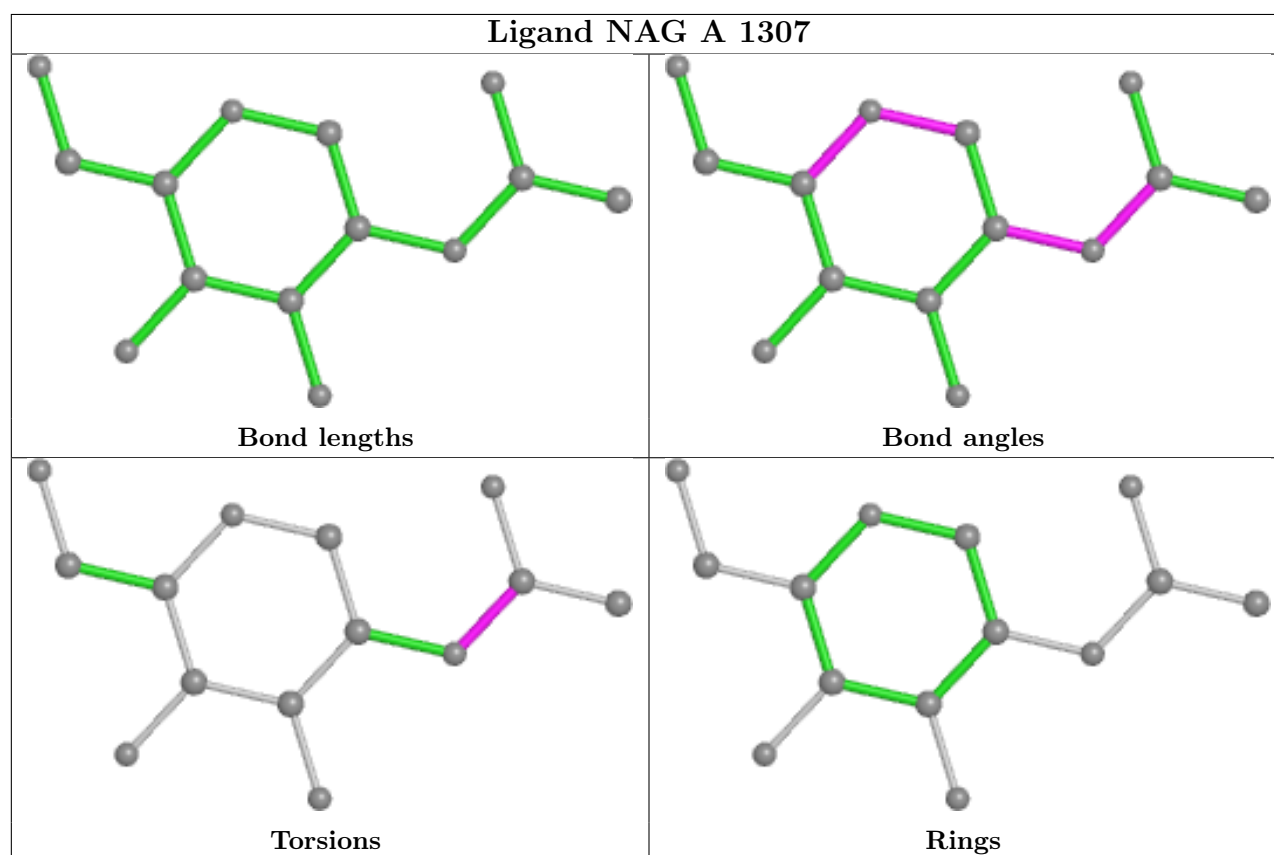
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1302	BLA	2	0

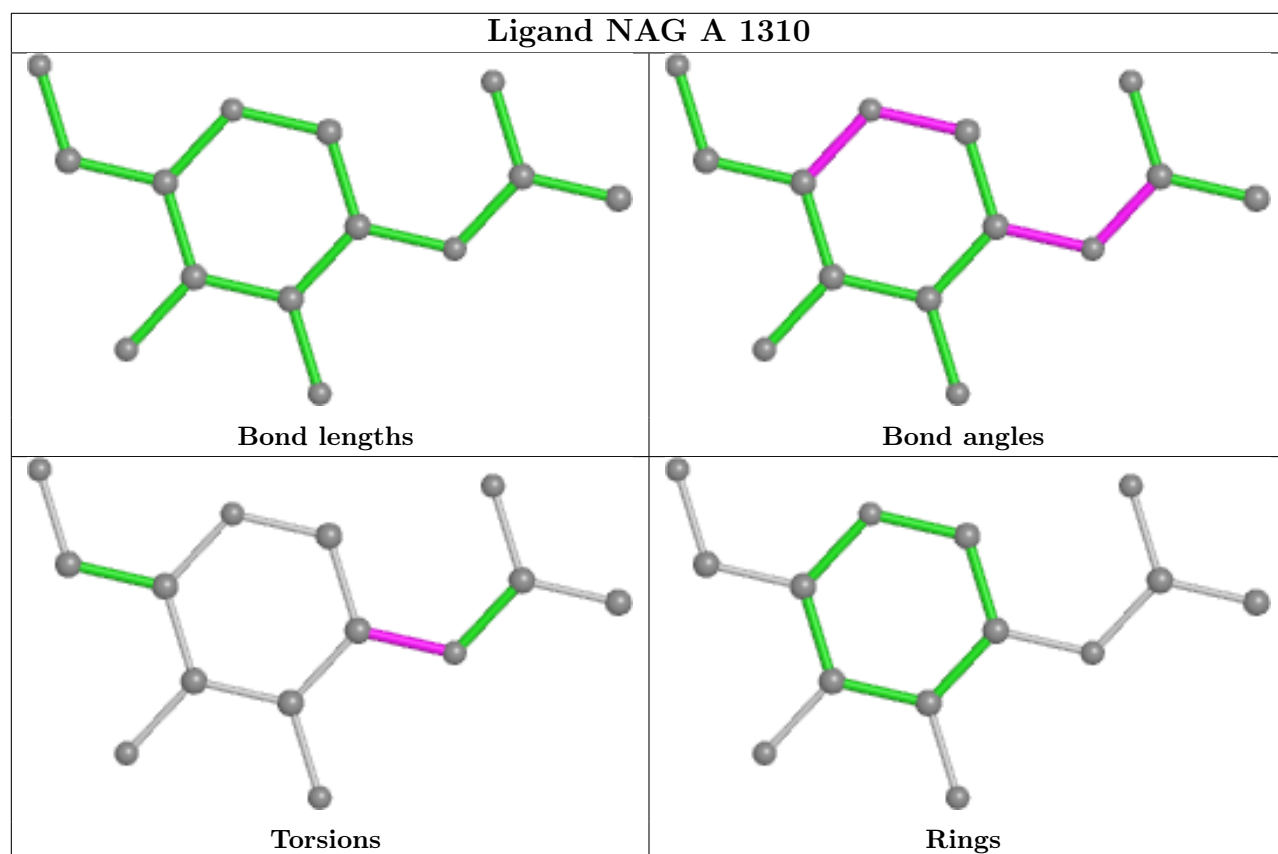
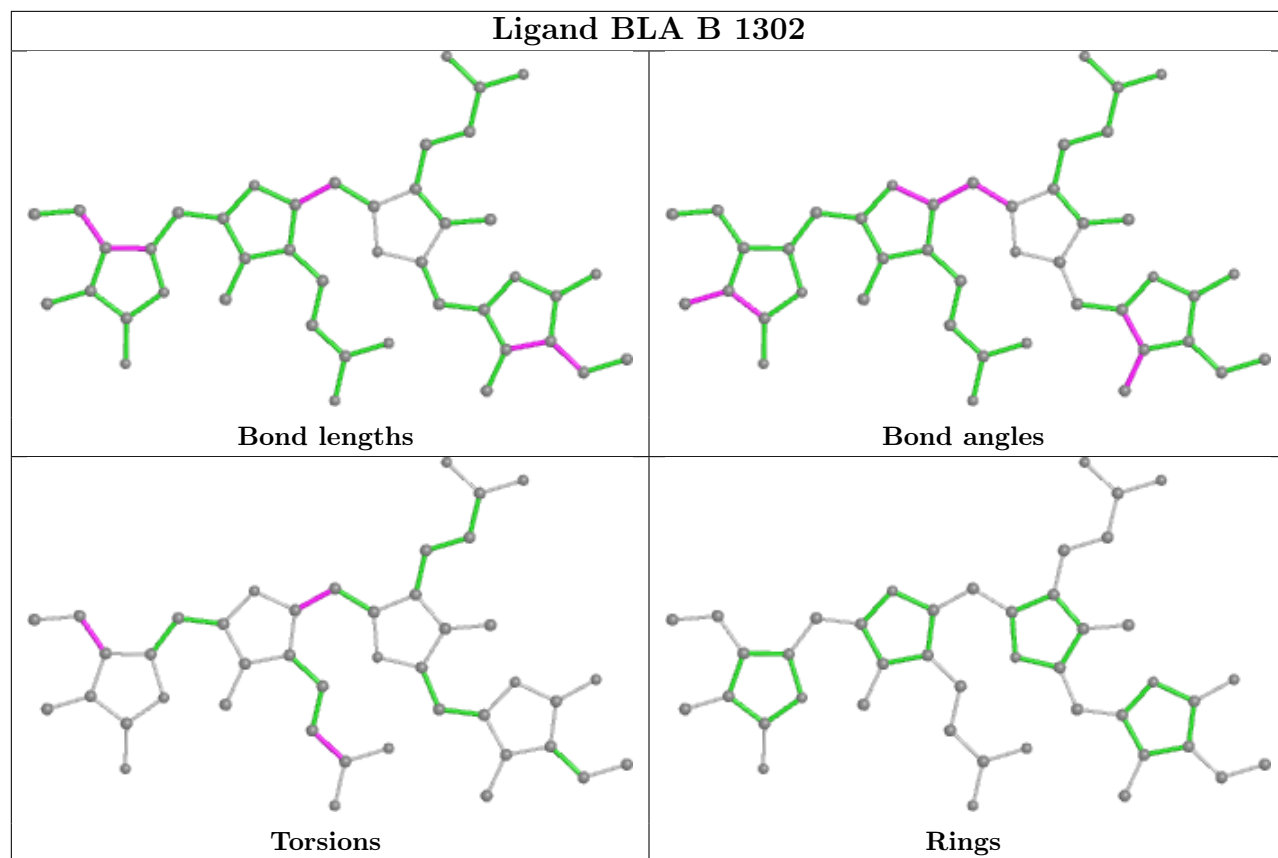
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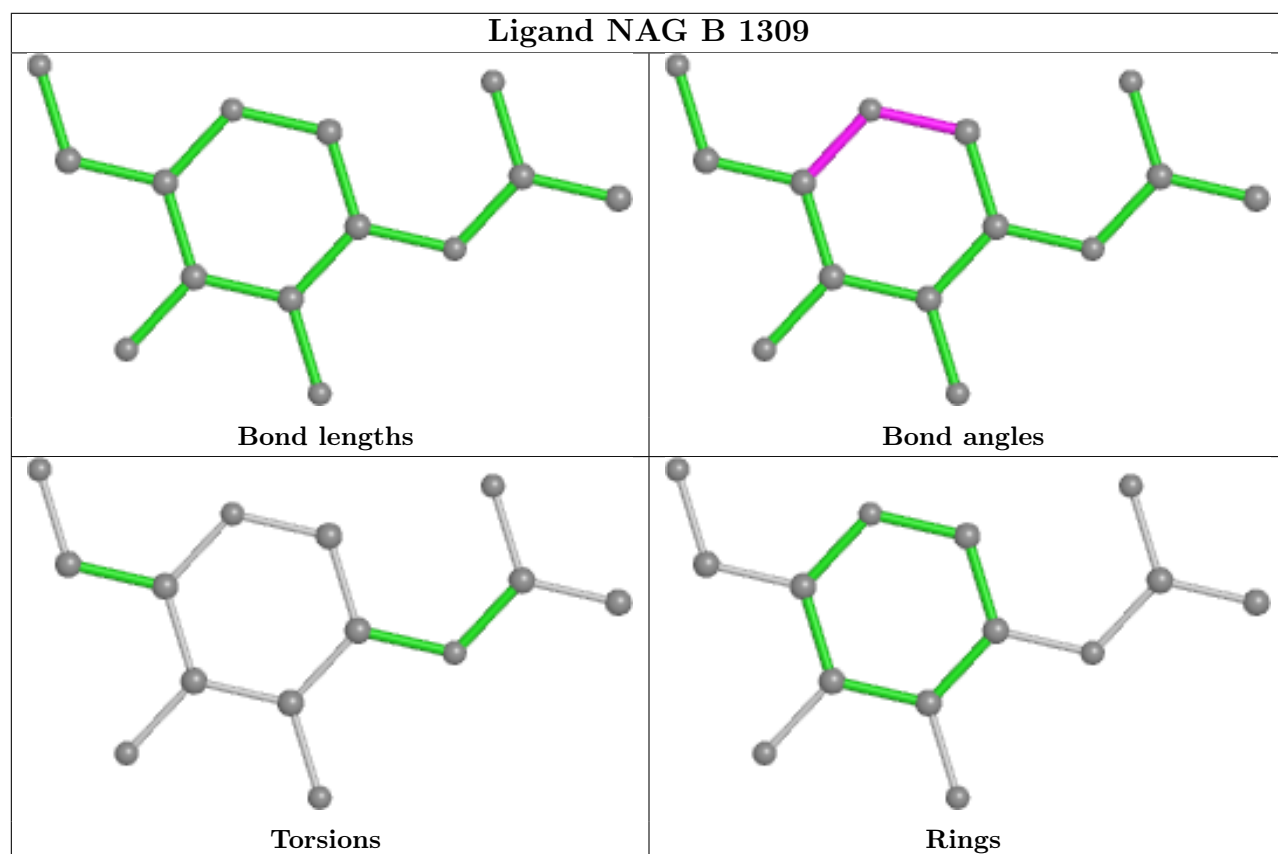
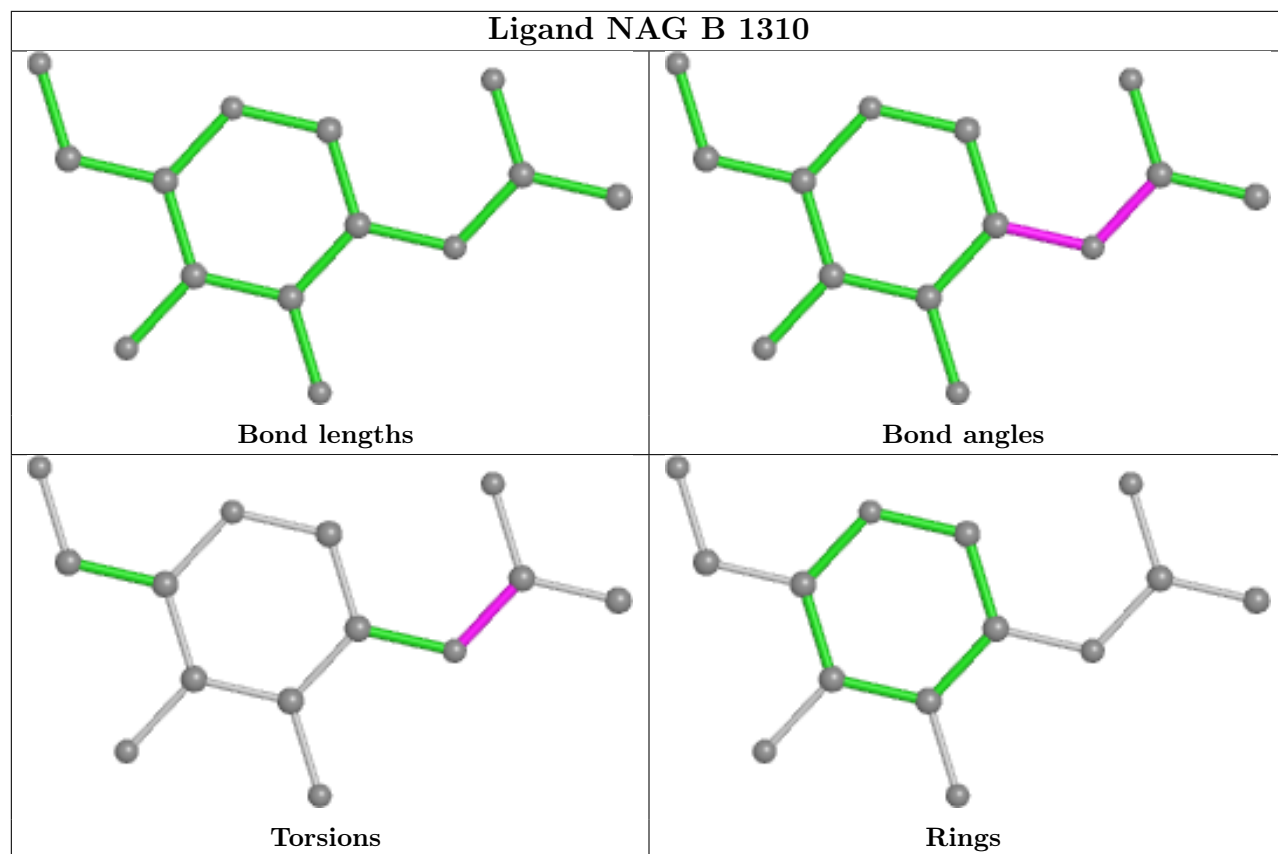
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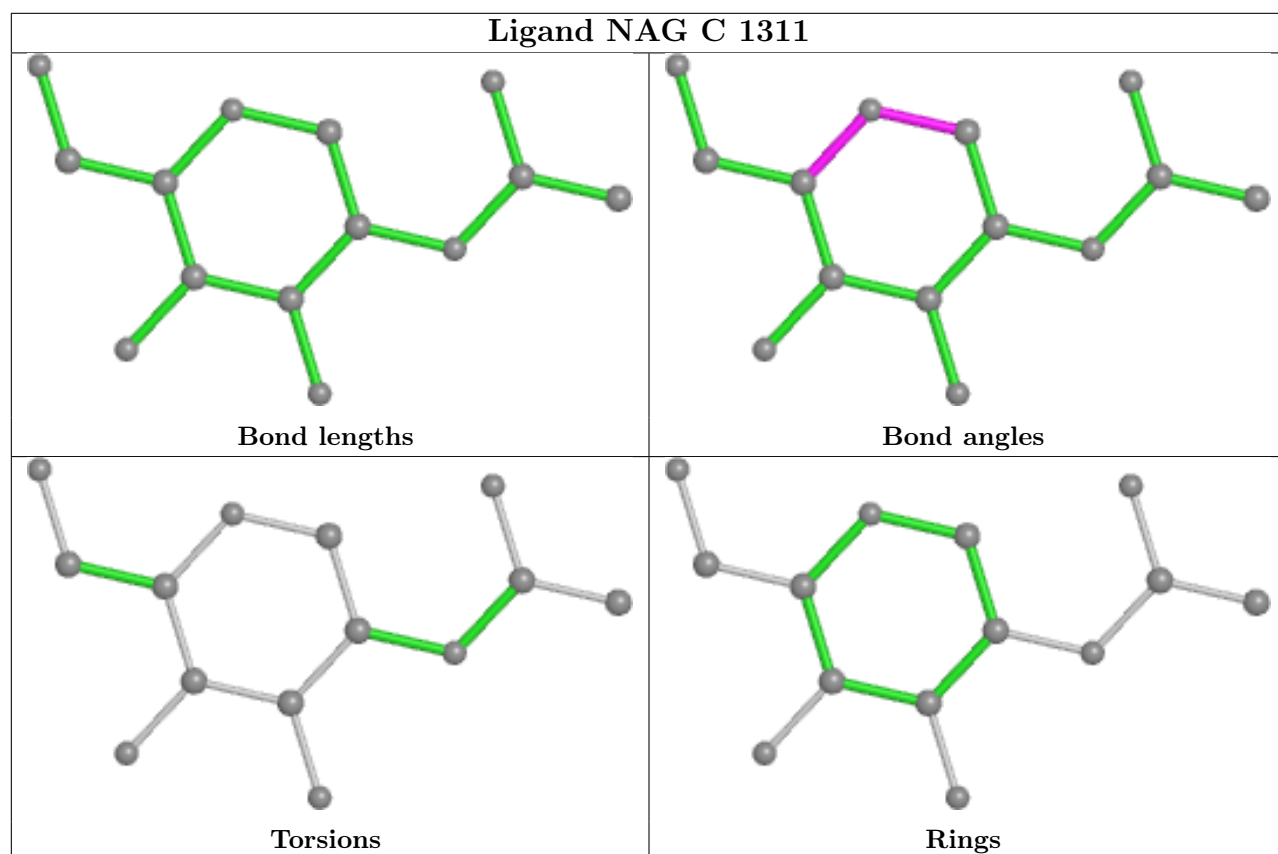
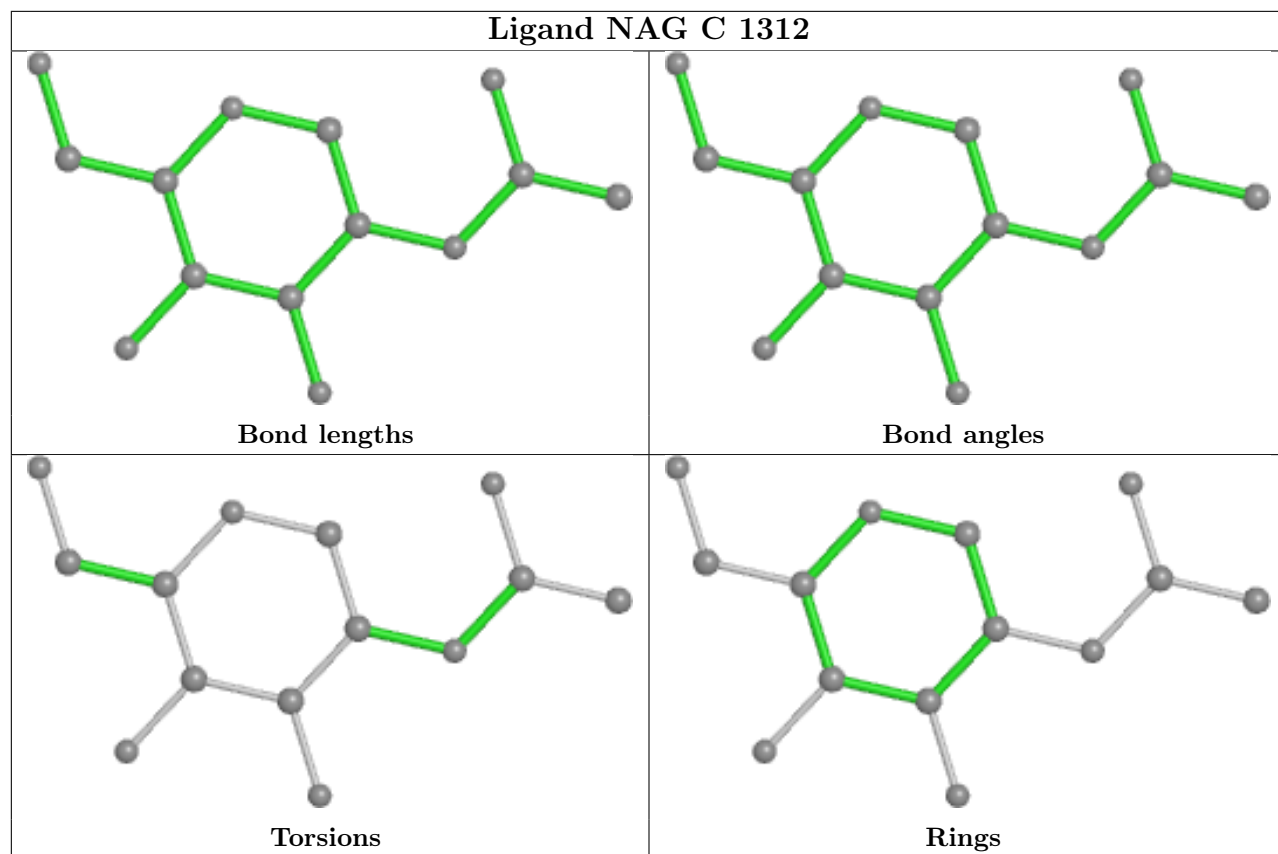
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1301	EIC	2	0
8	A	1313	EIC	1	0
8	C	1301	EIC	2	0
6	A	1301	BLA	1	0

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

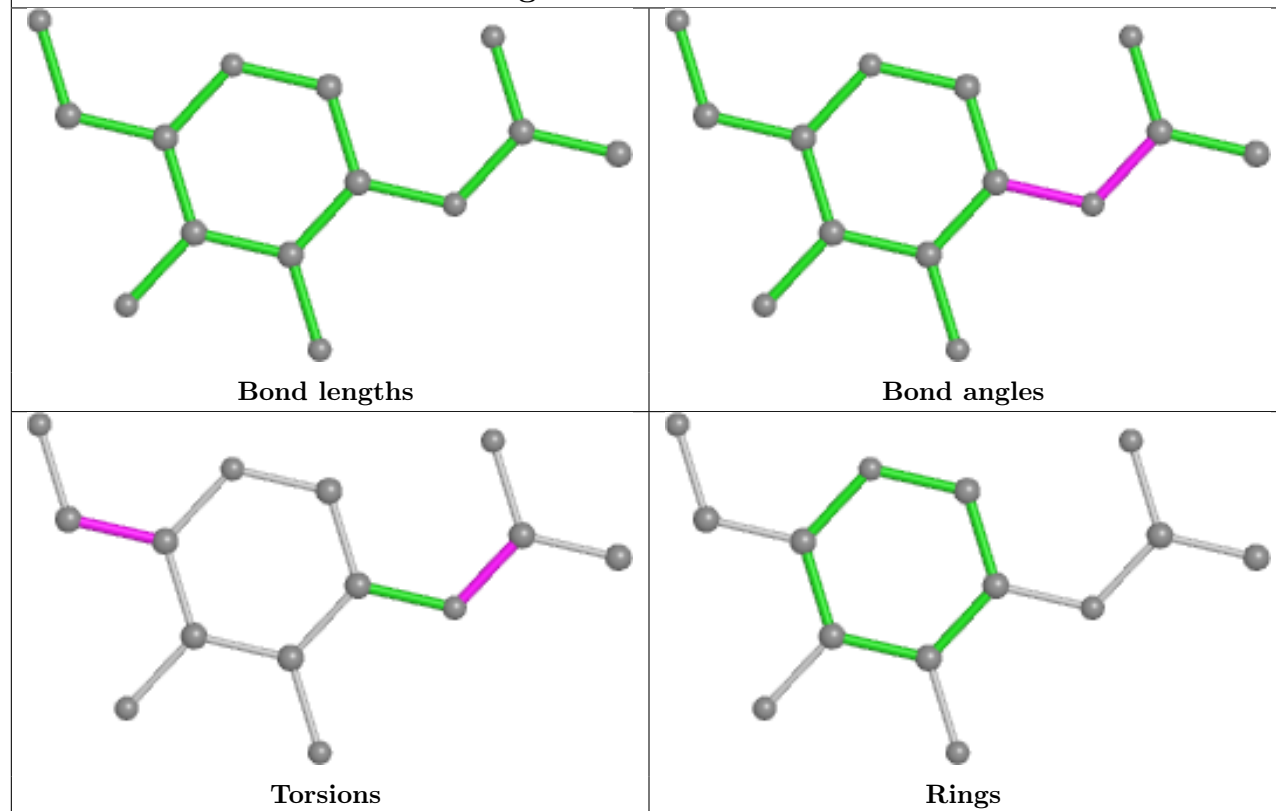




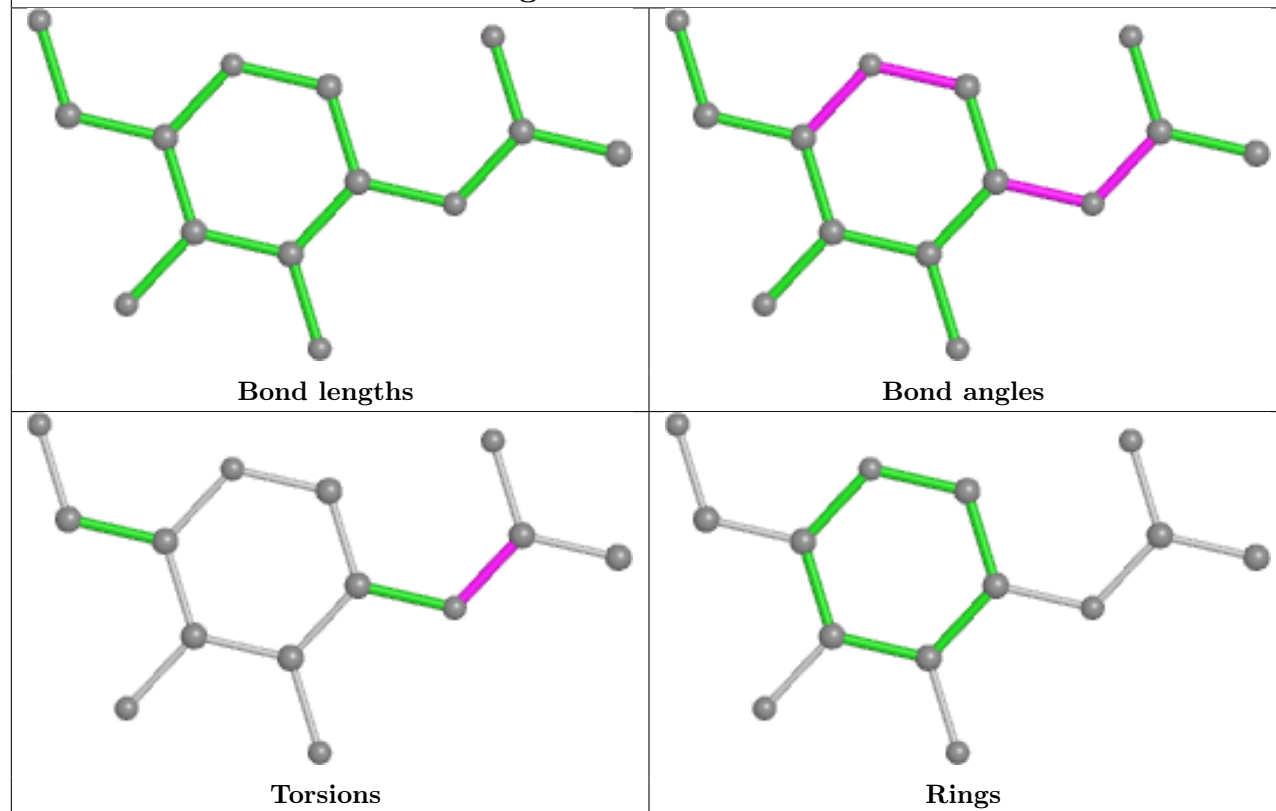


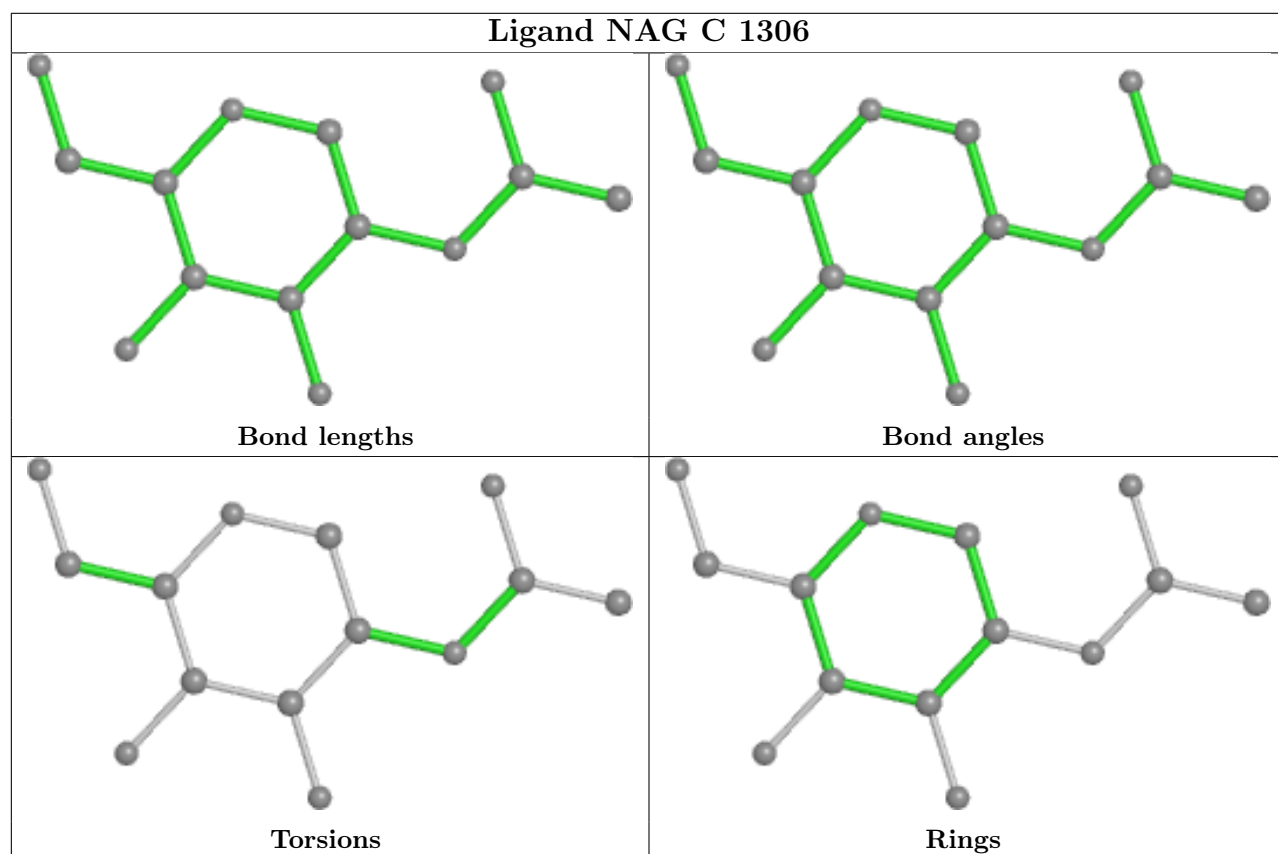
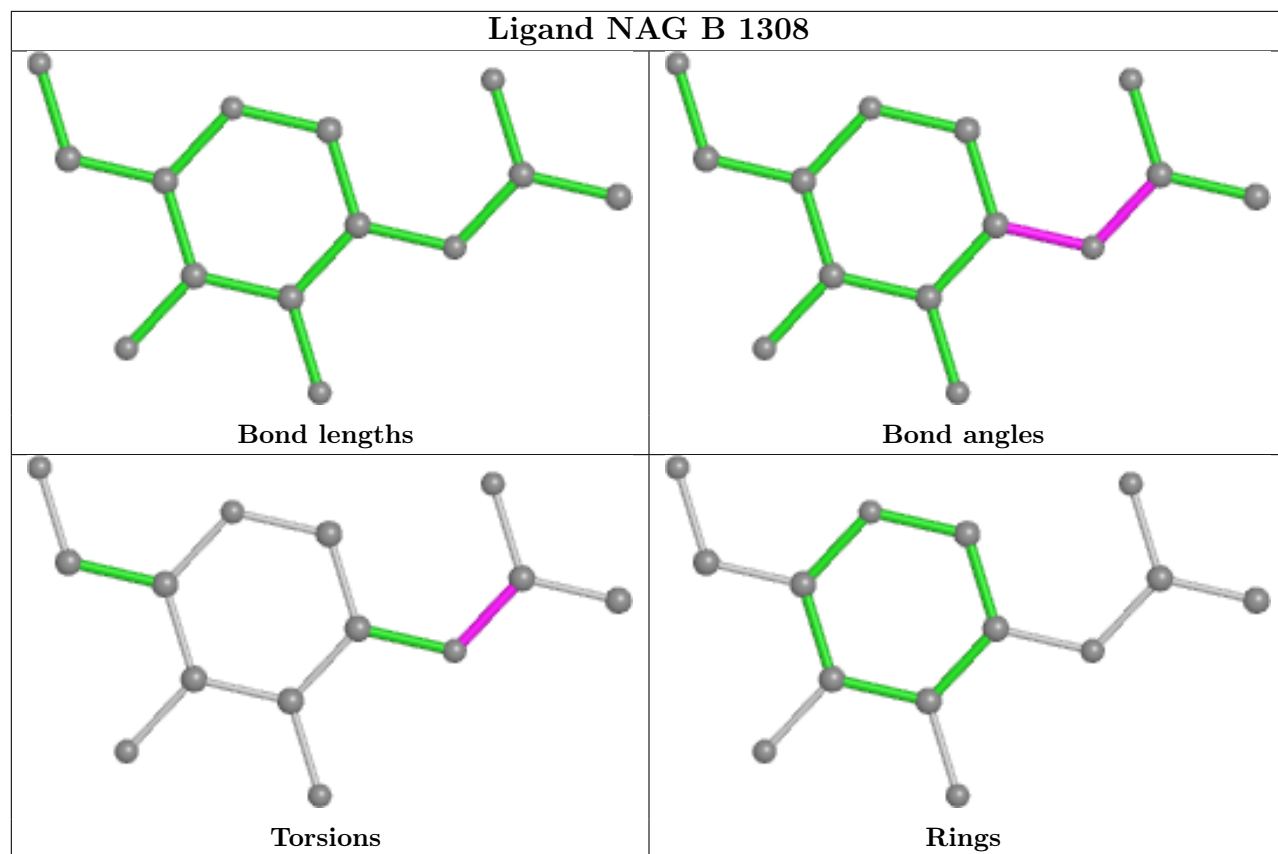


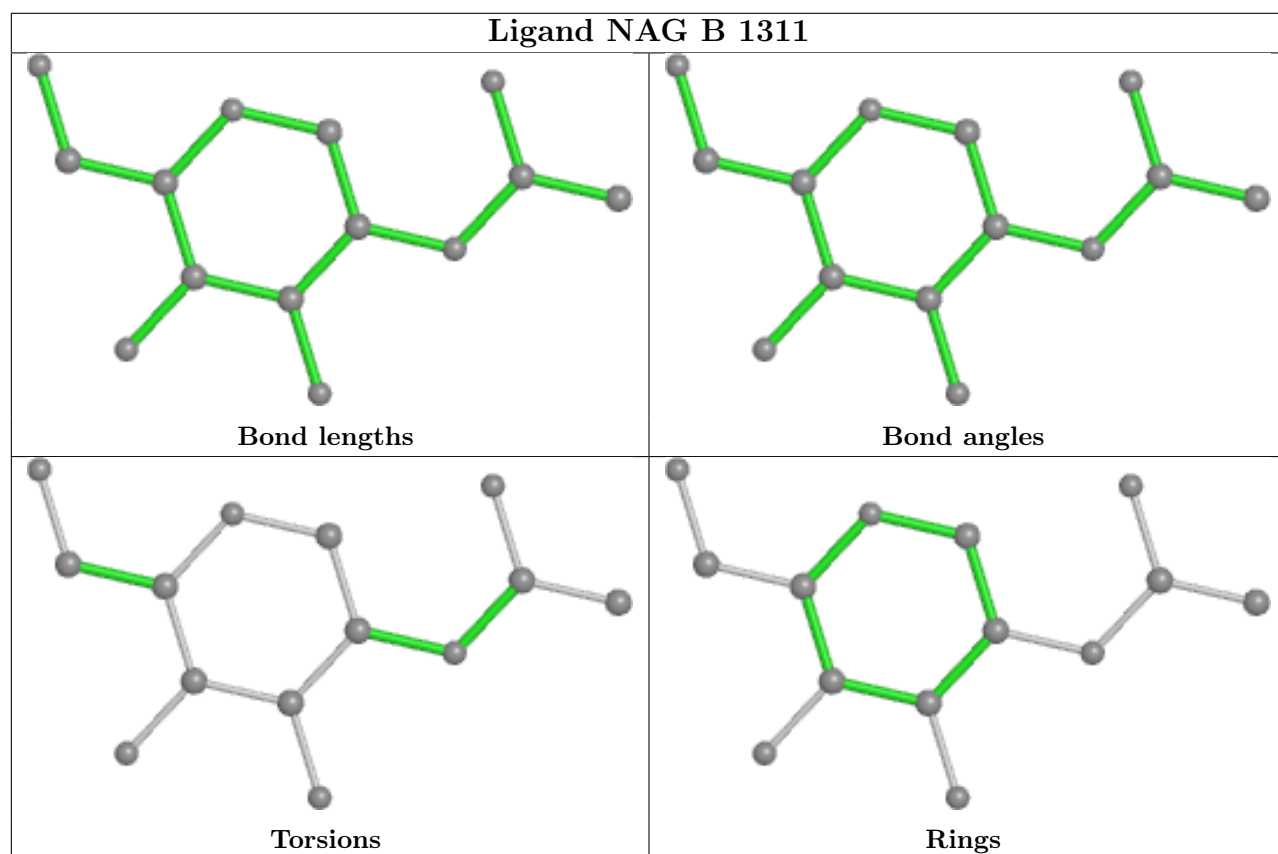
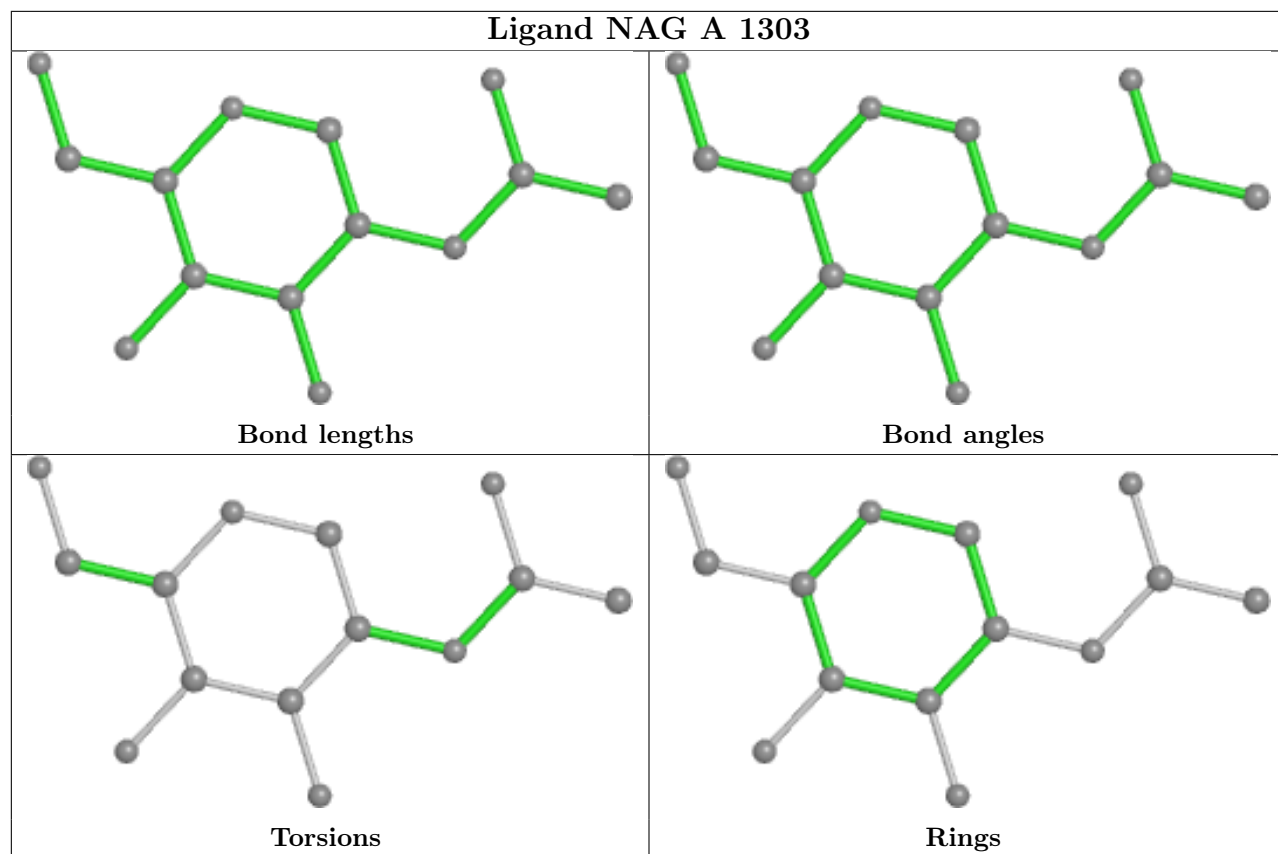
Ligand NAG A 1304

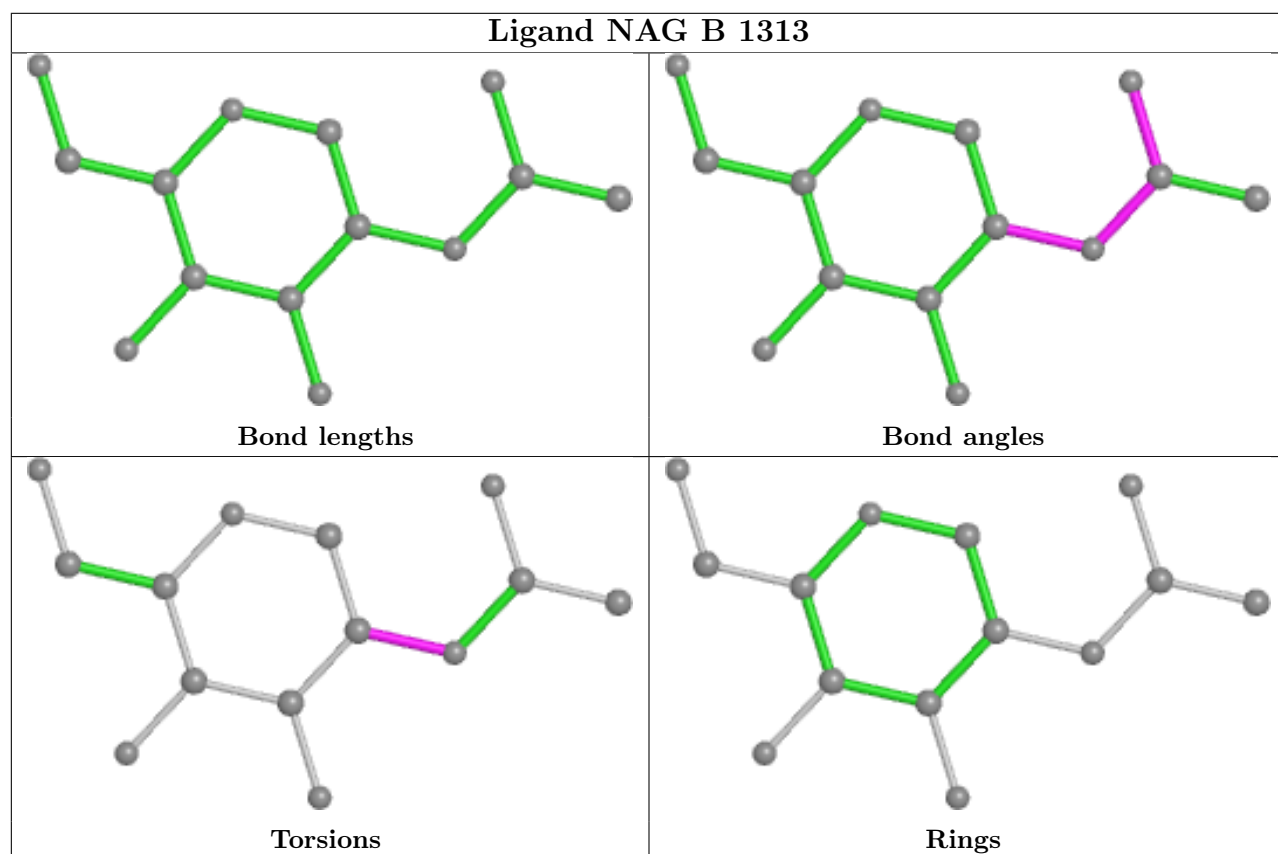
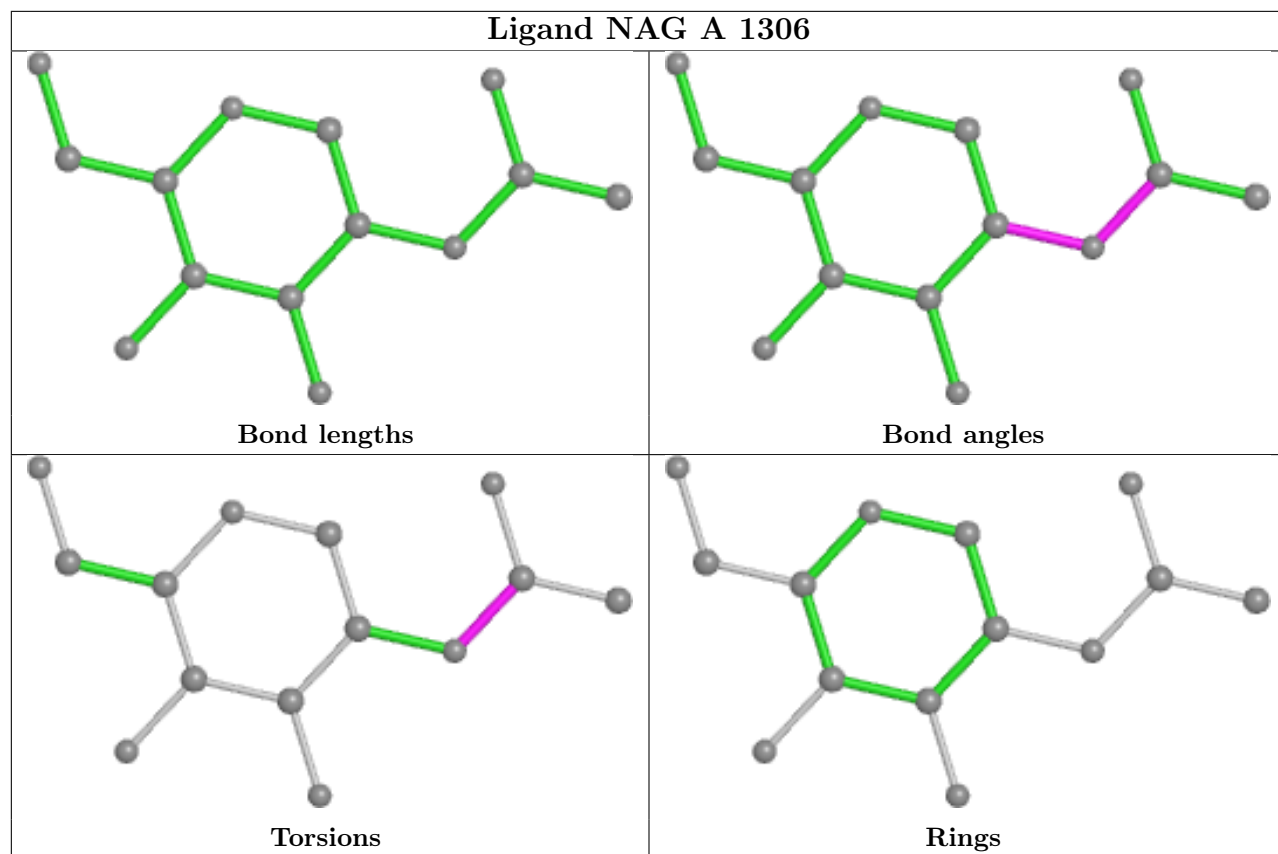


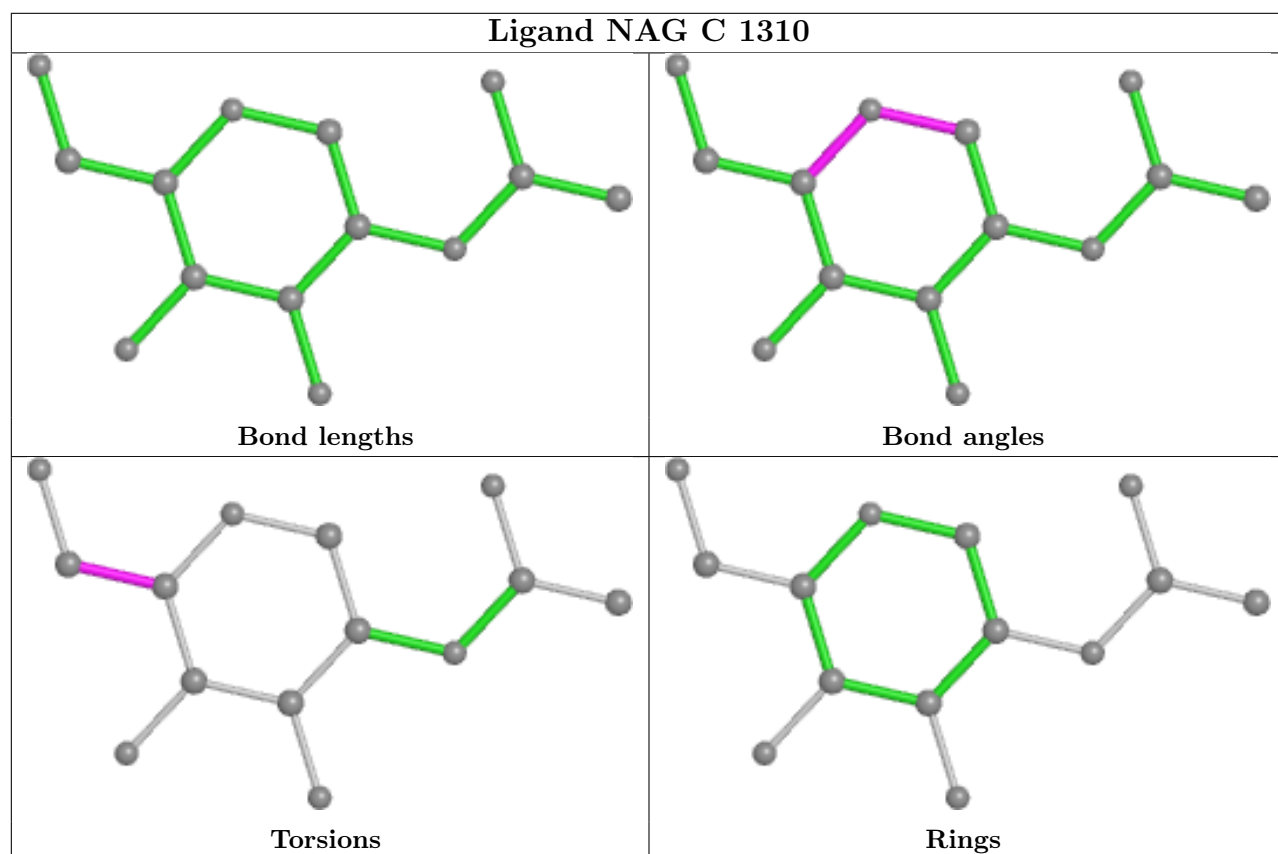
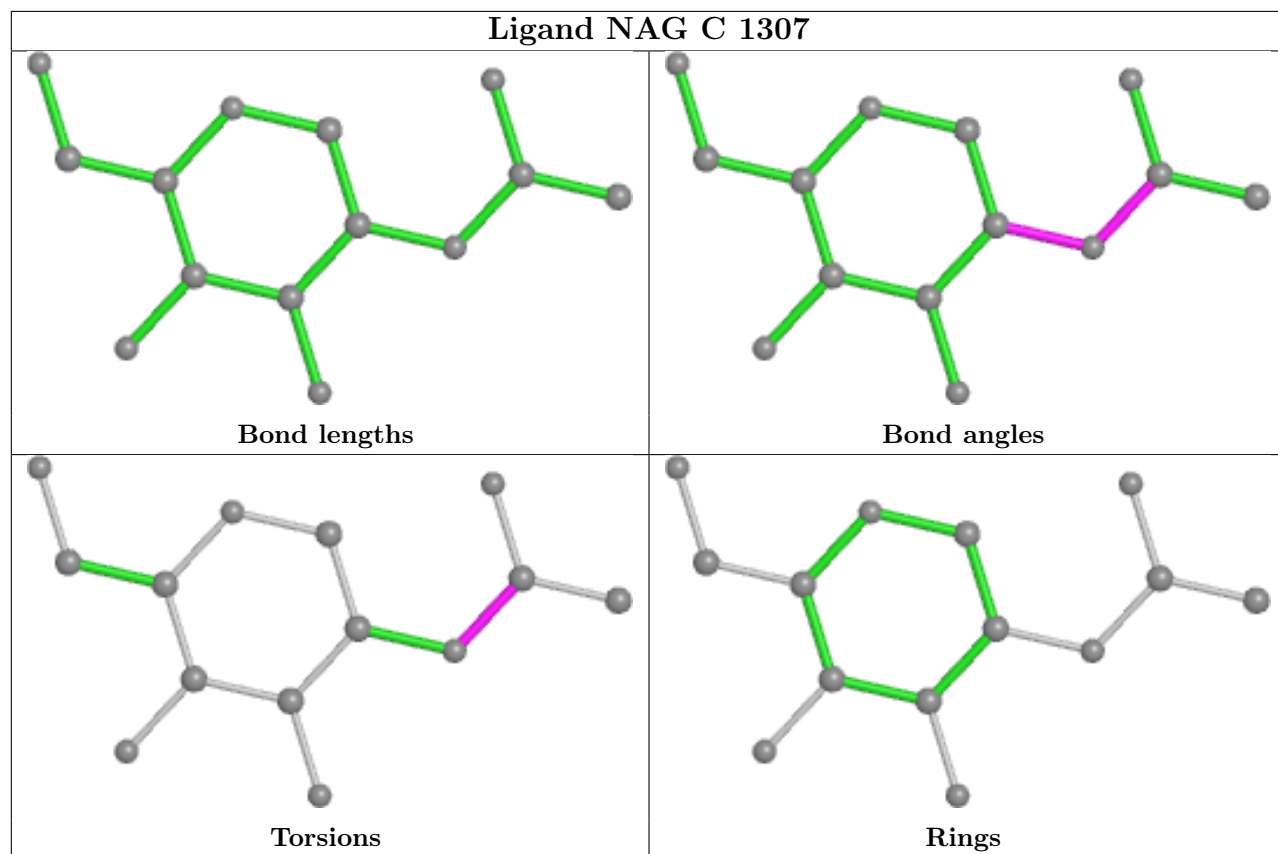
Ligand NAG C 1313



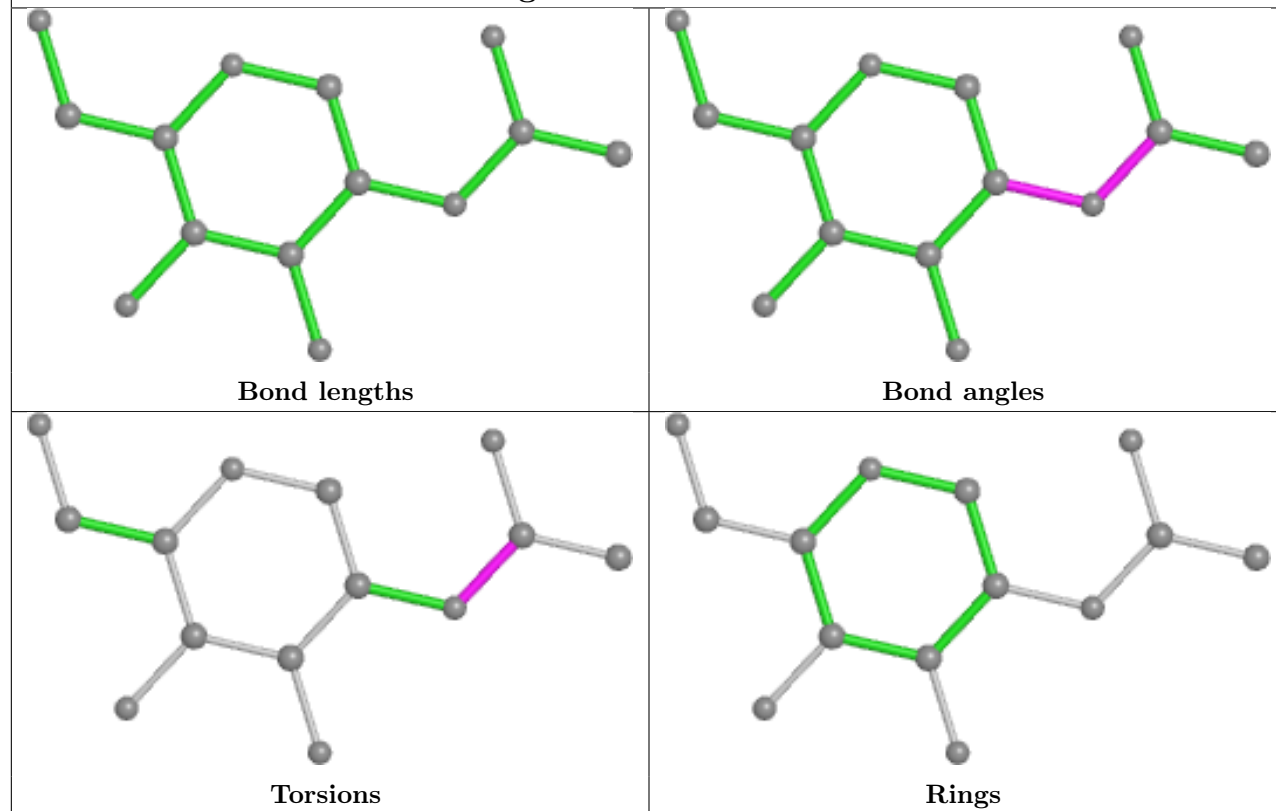




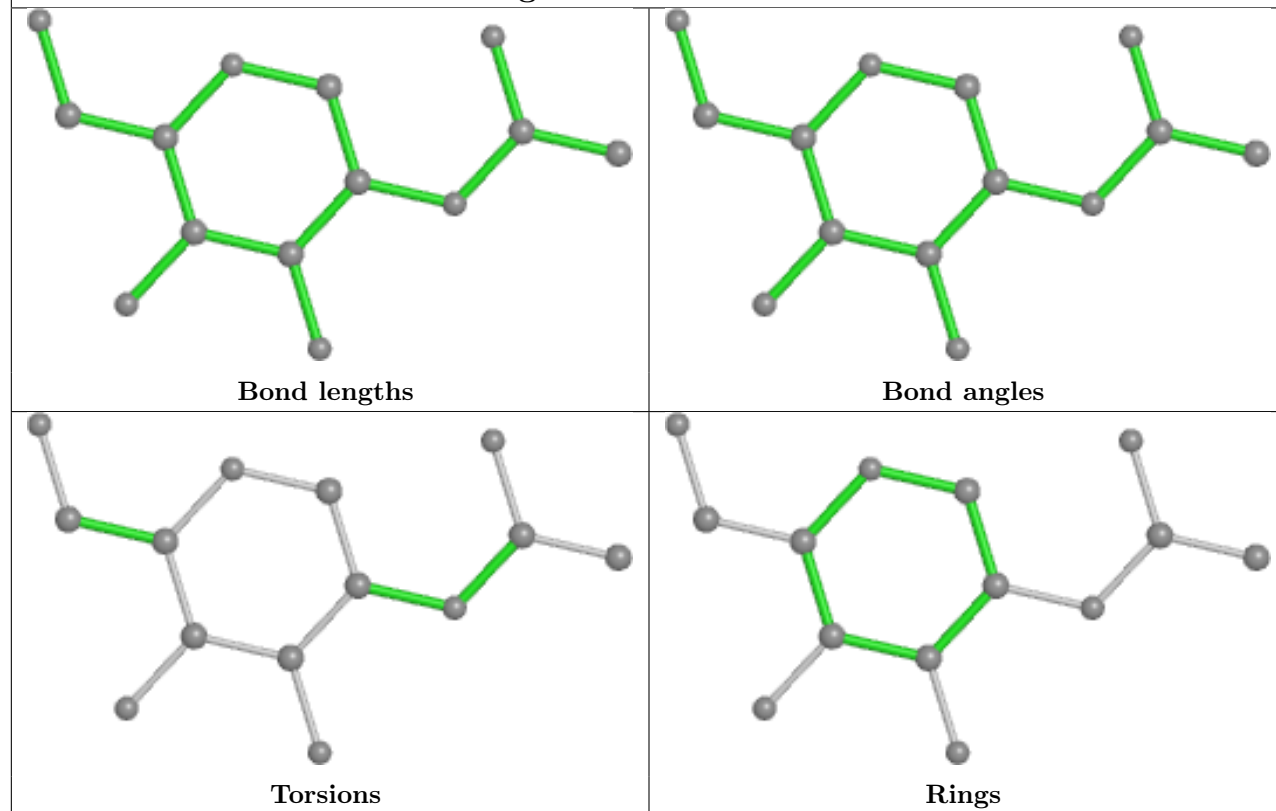


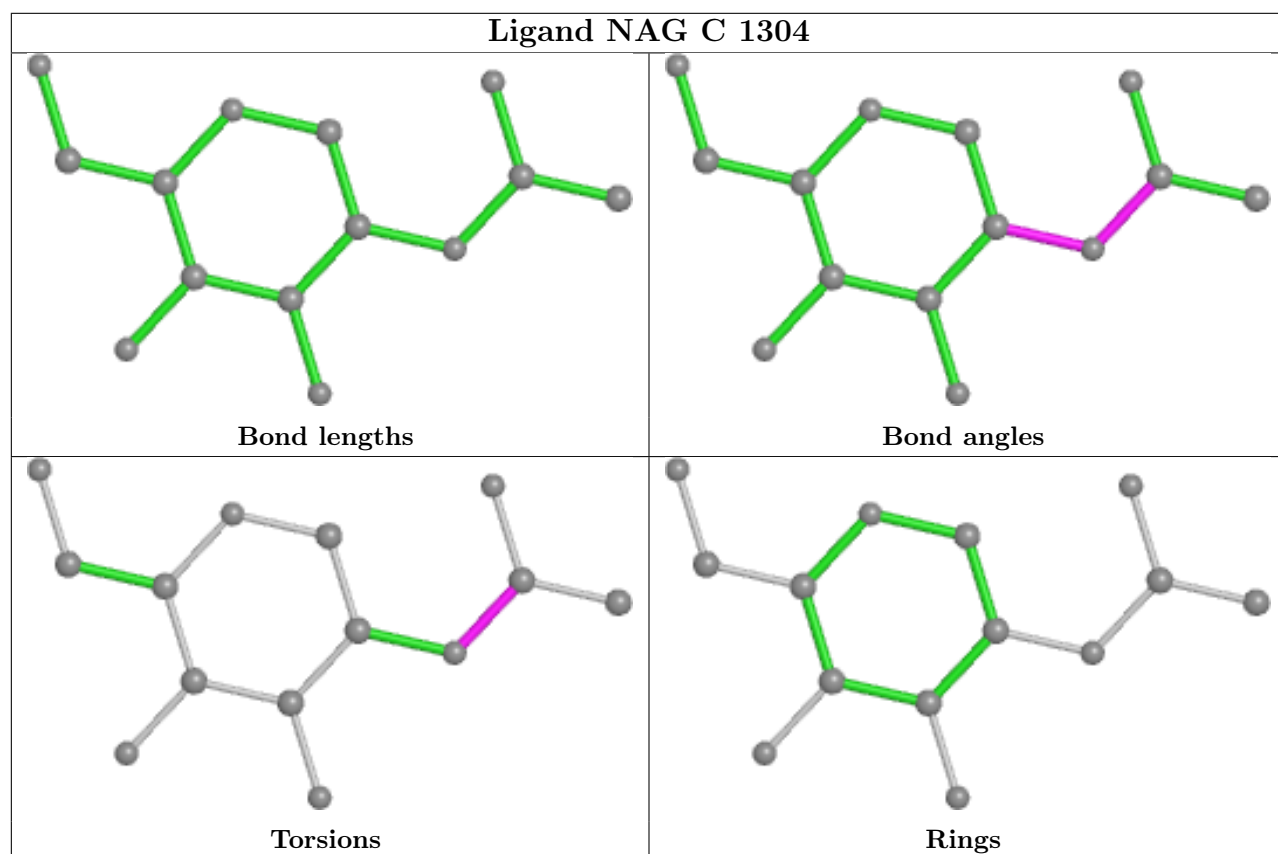
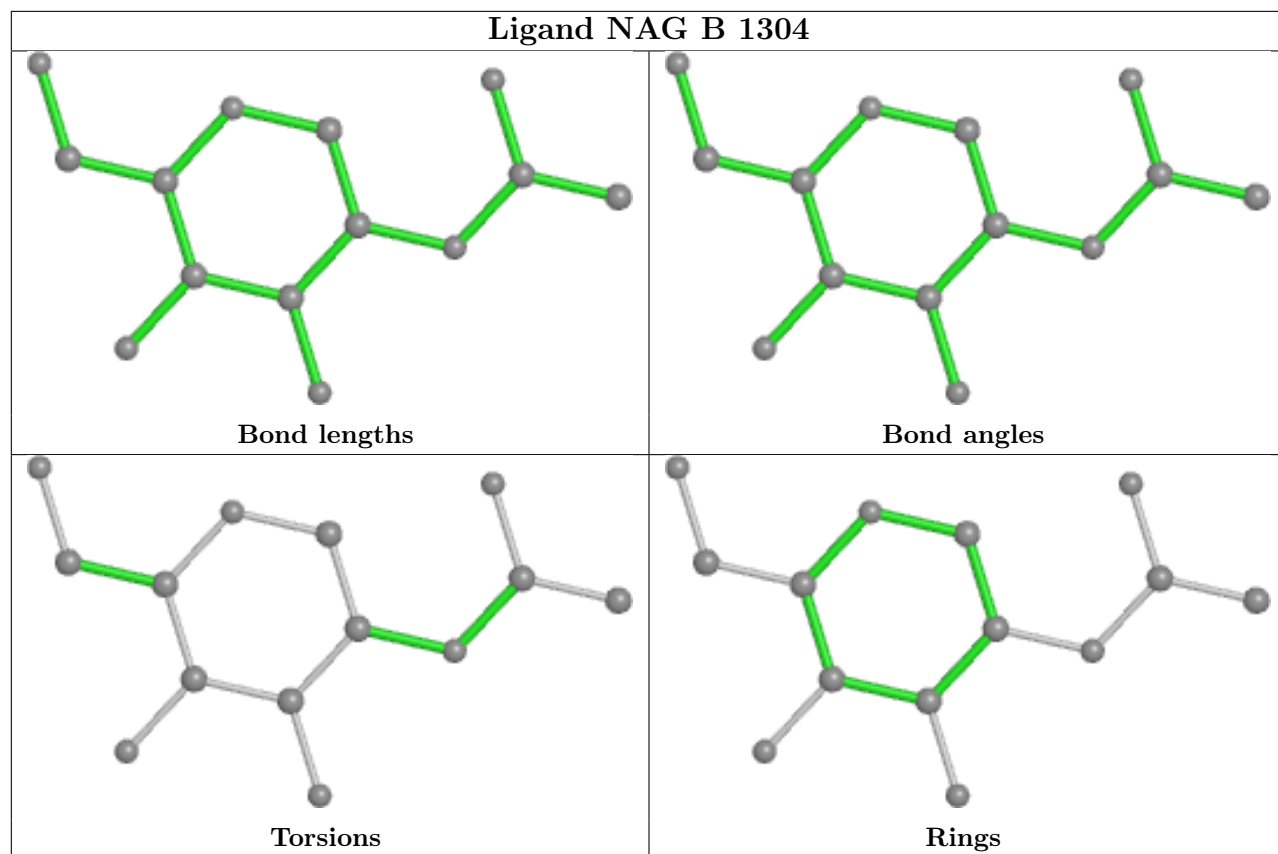


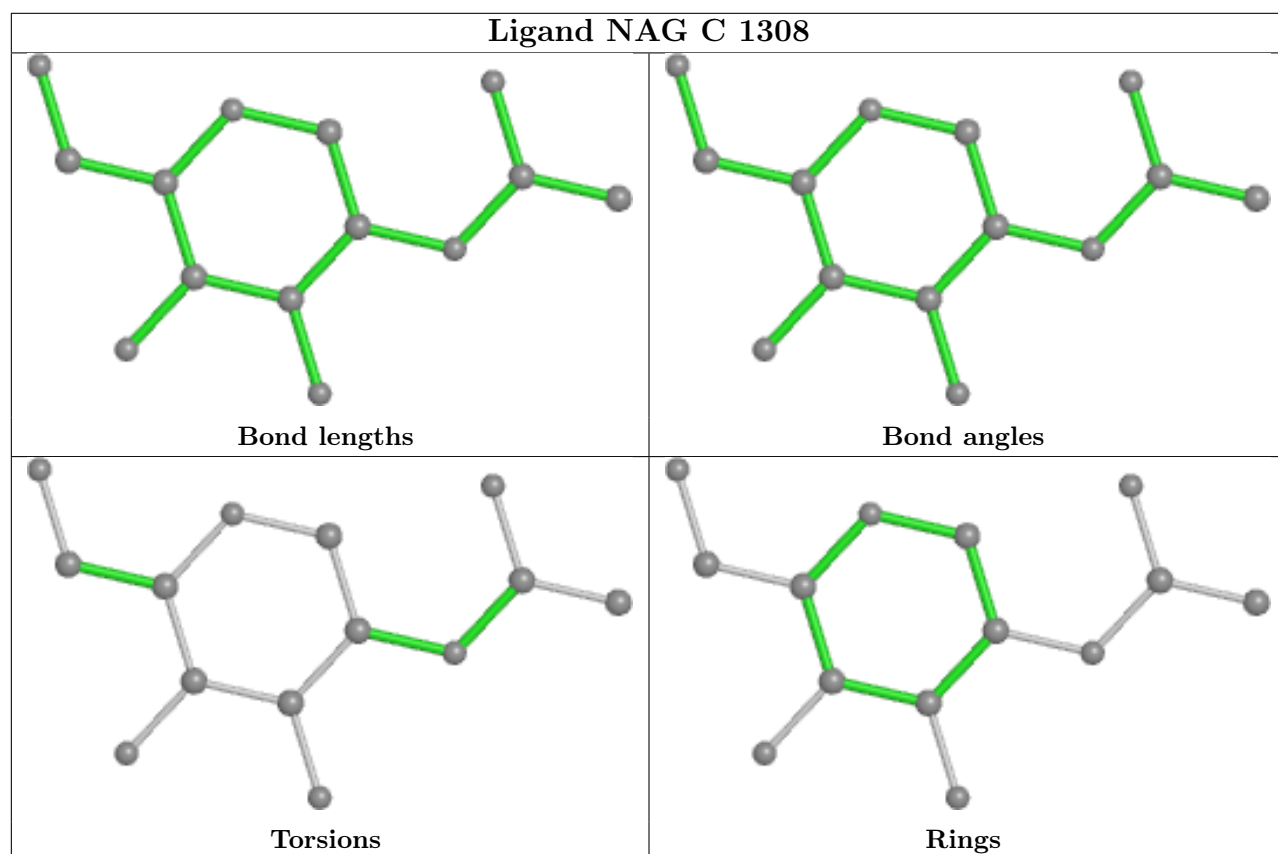
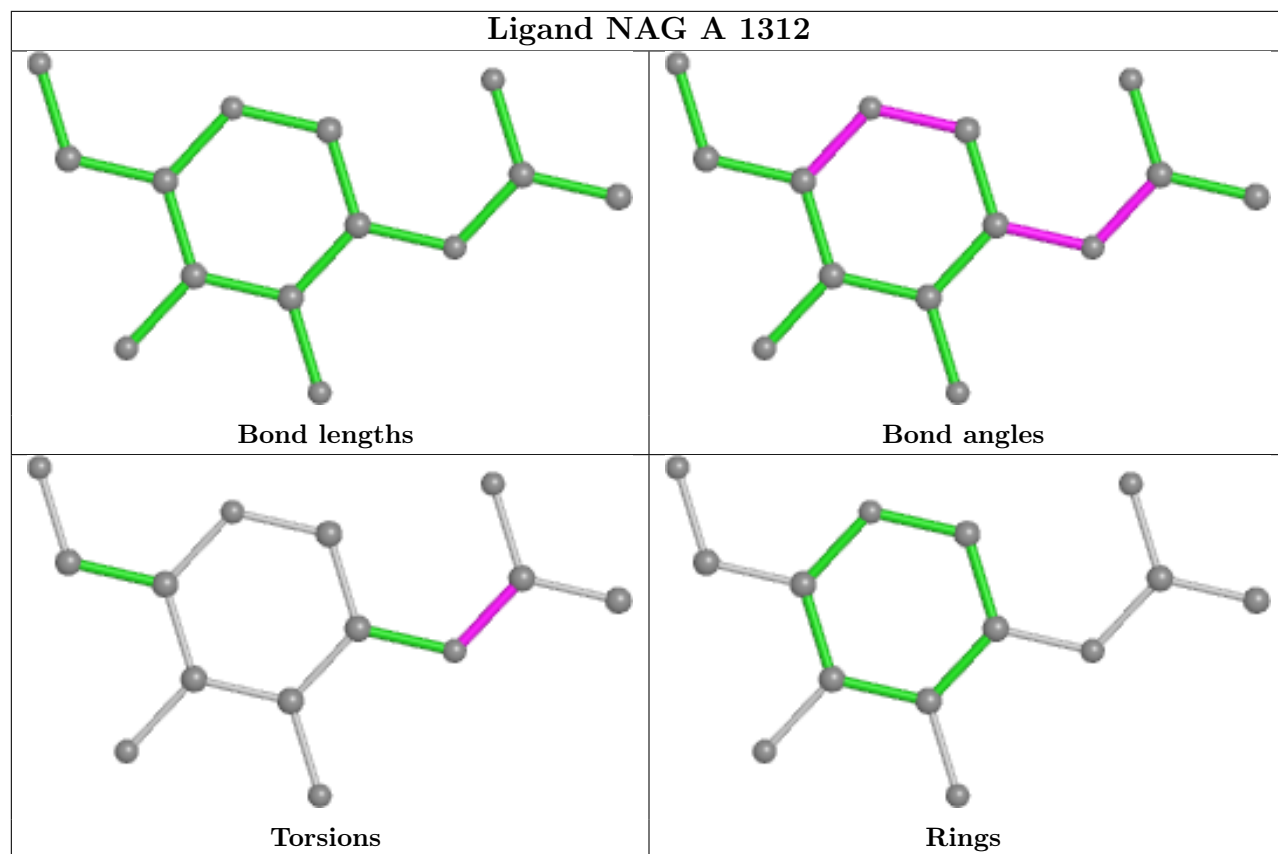
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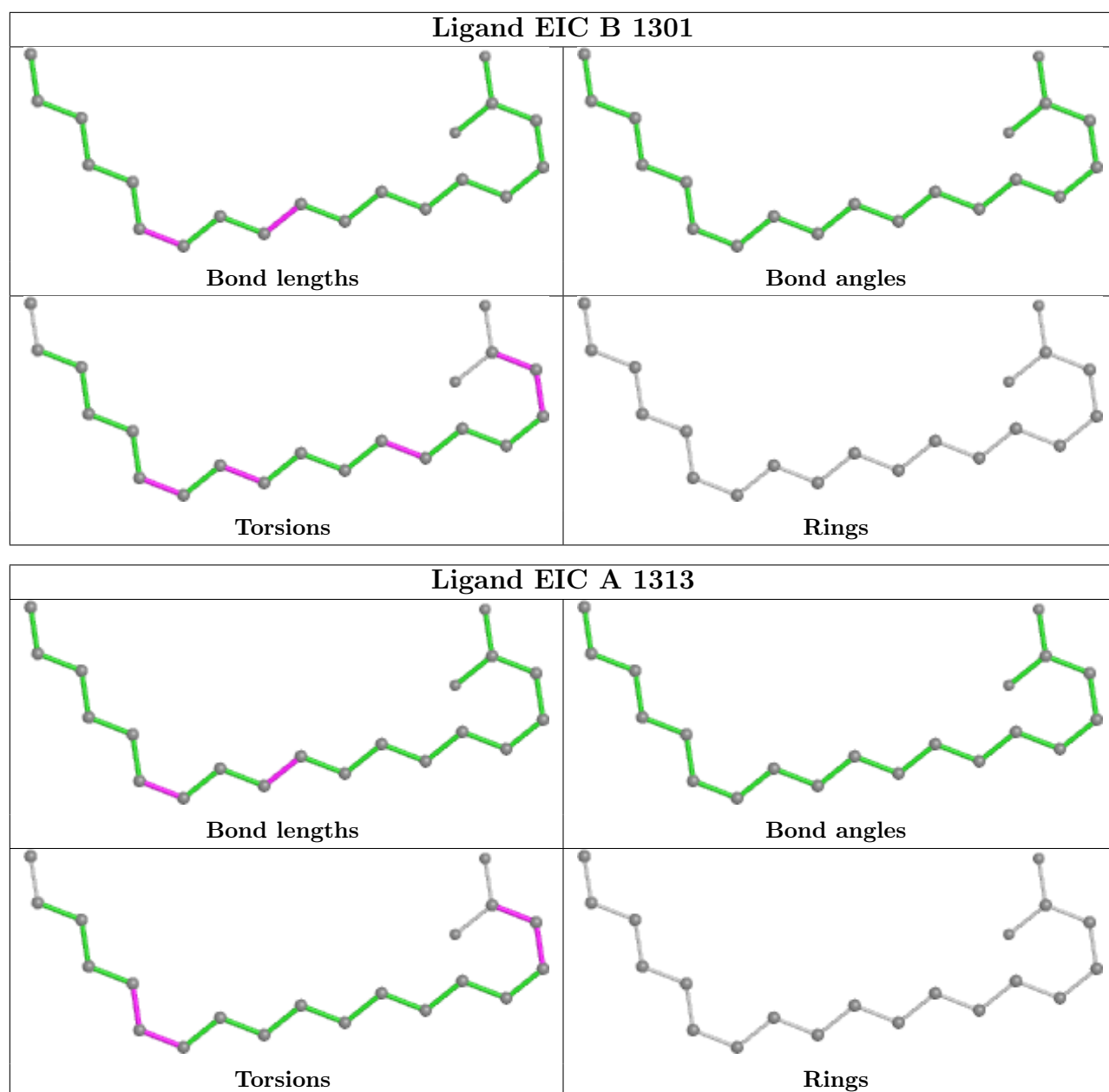


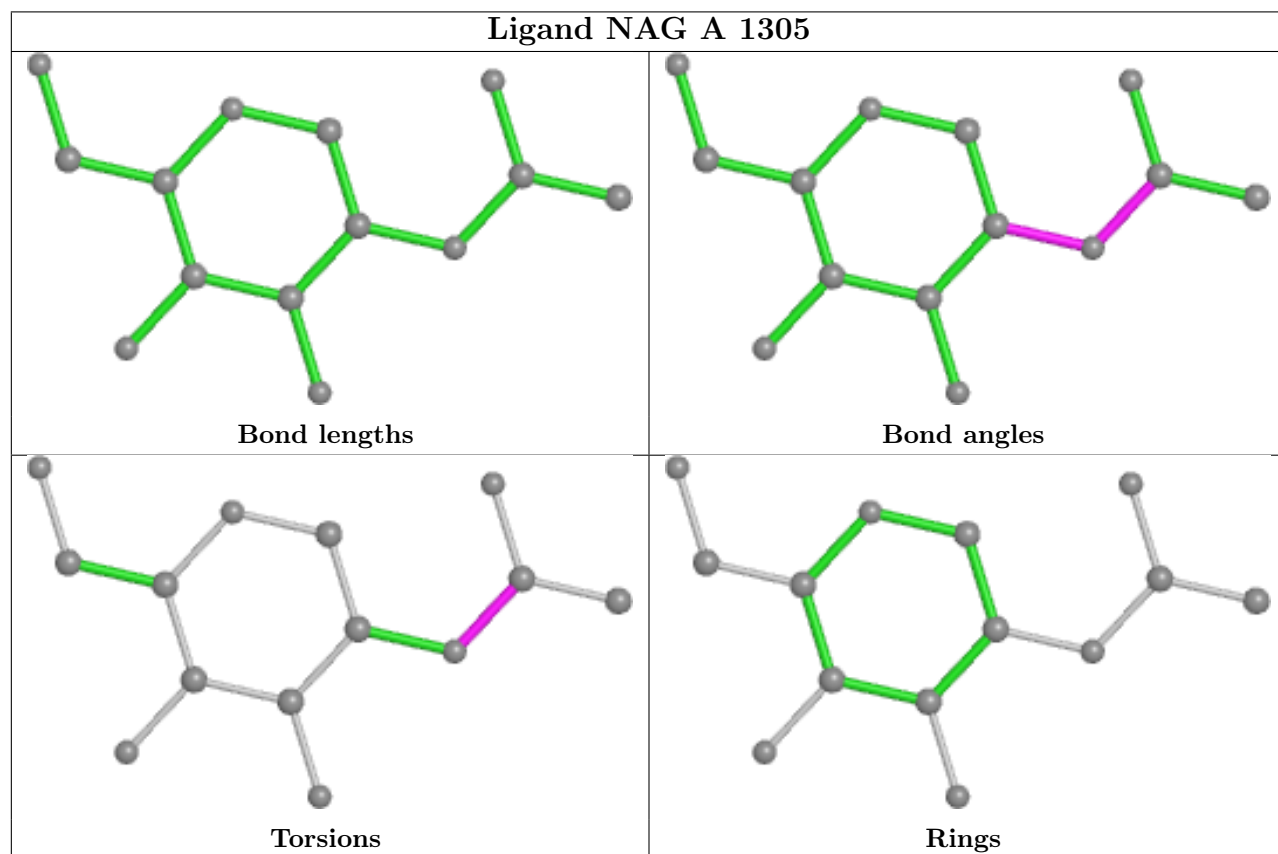
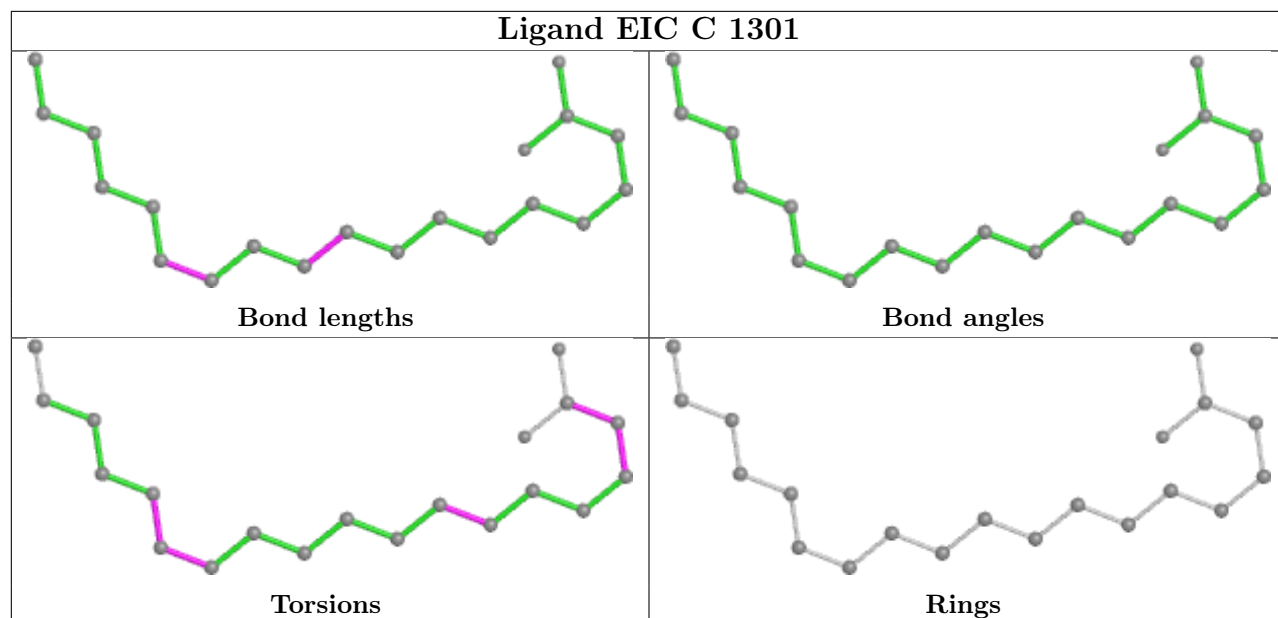
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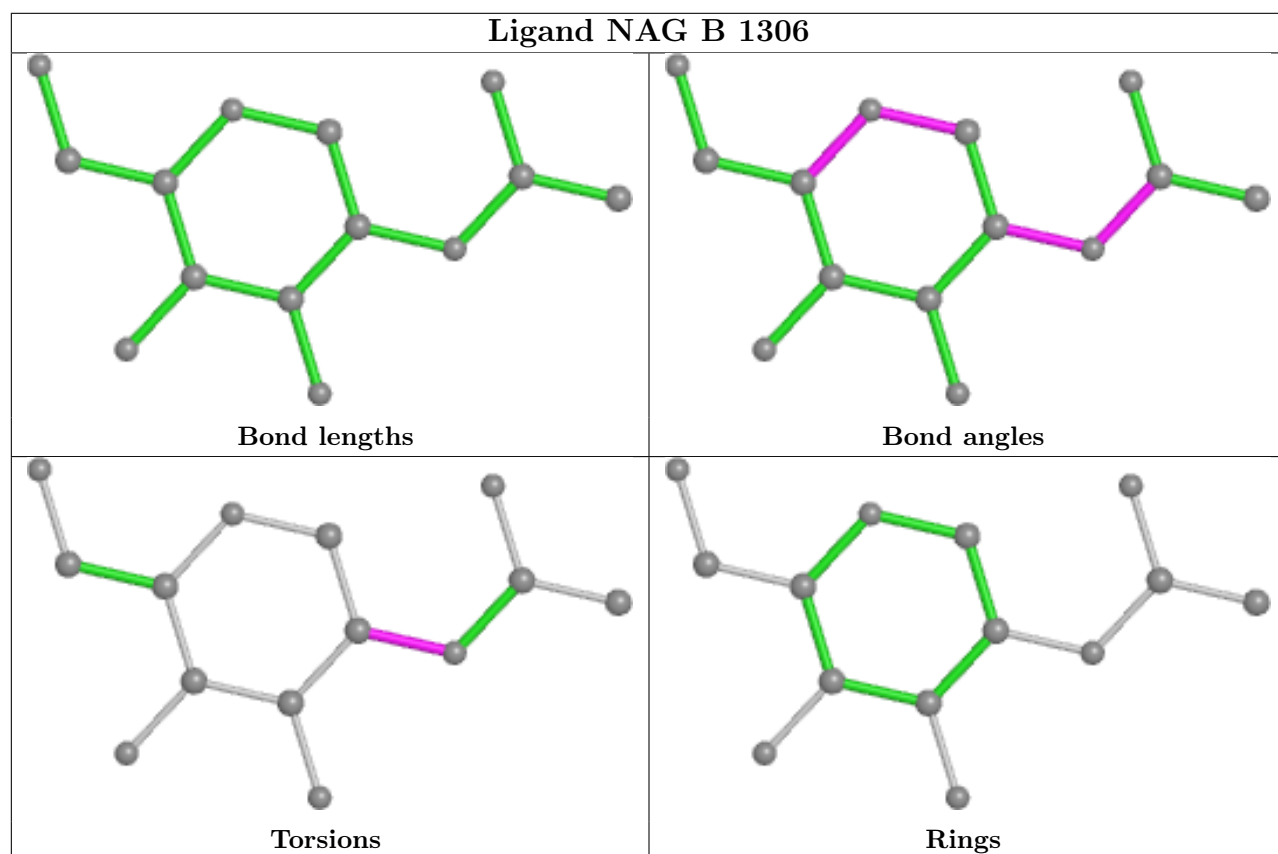
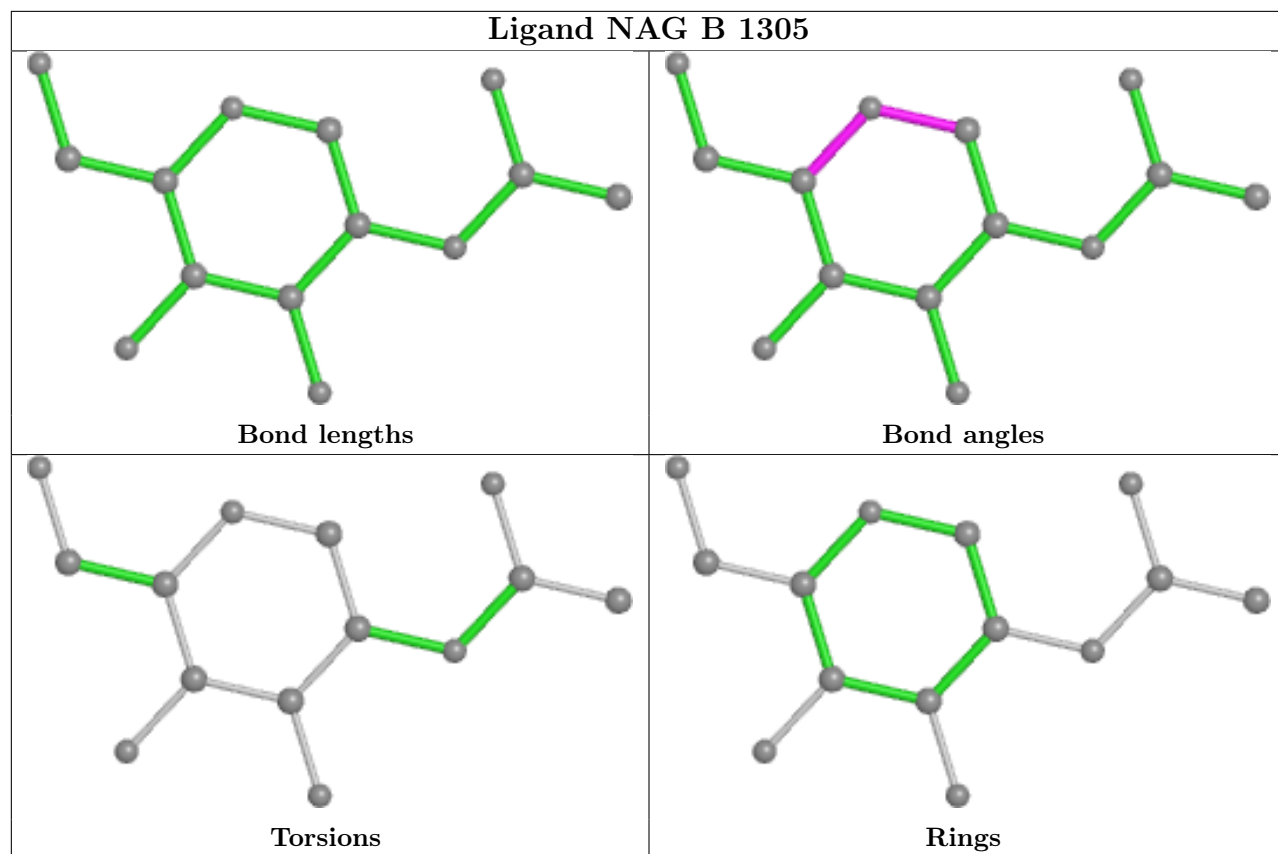


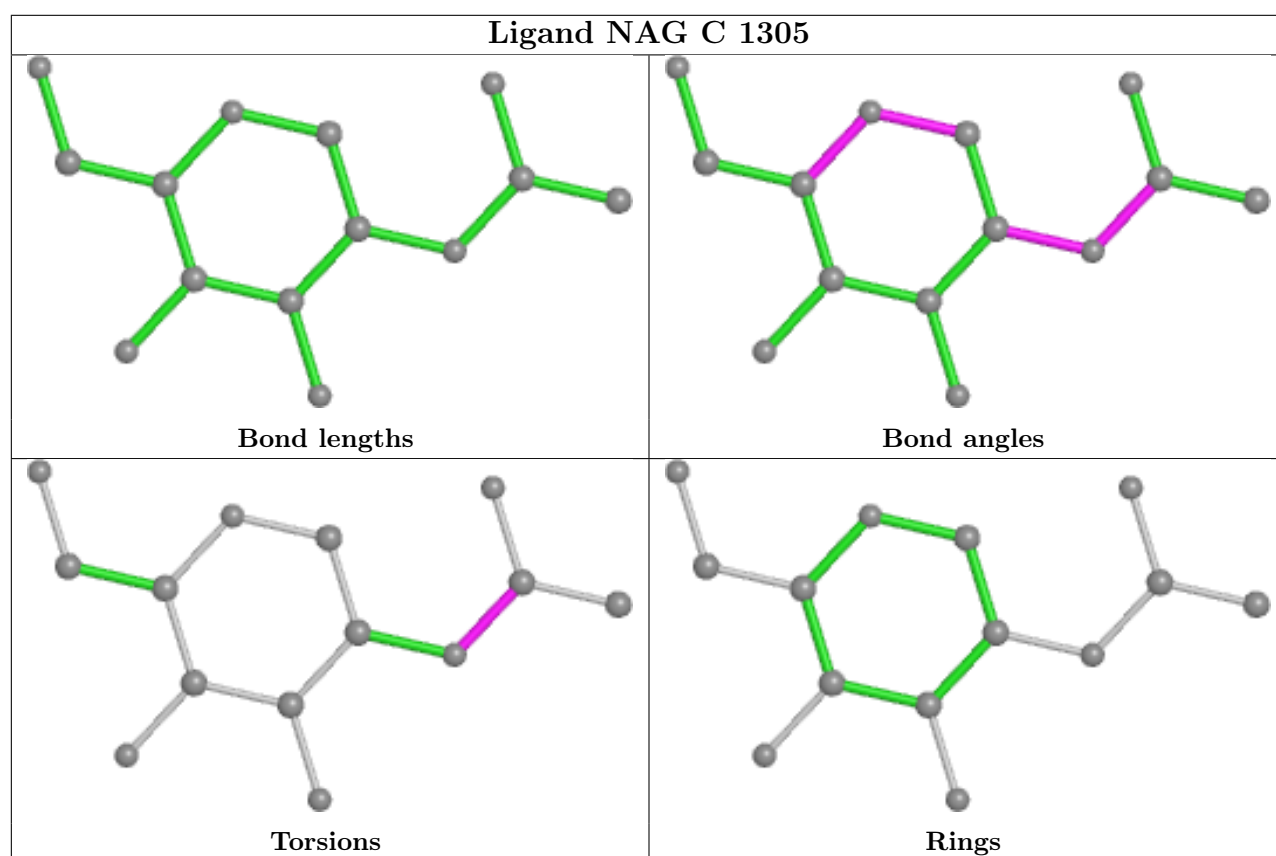
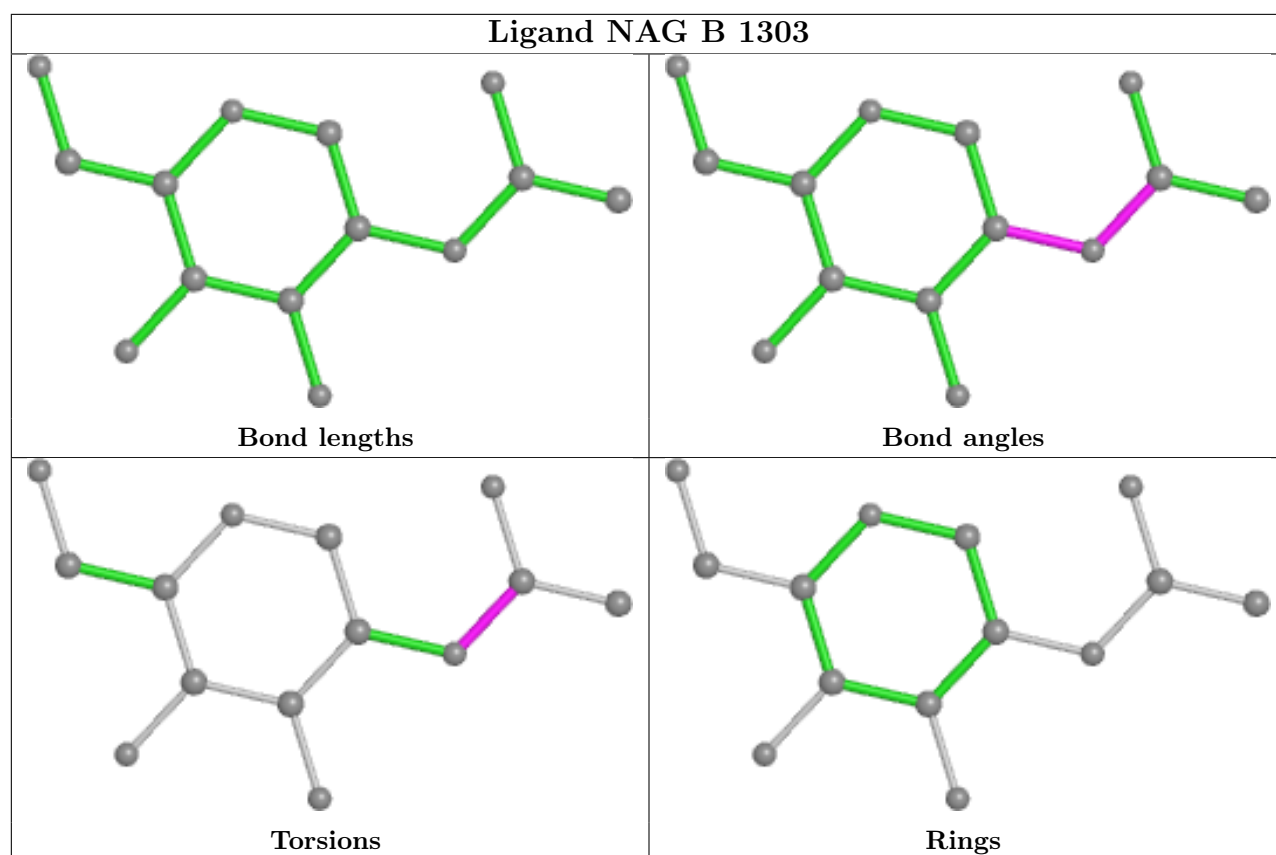




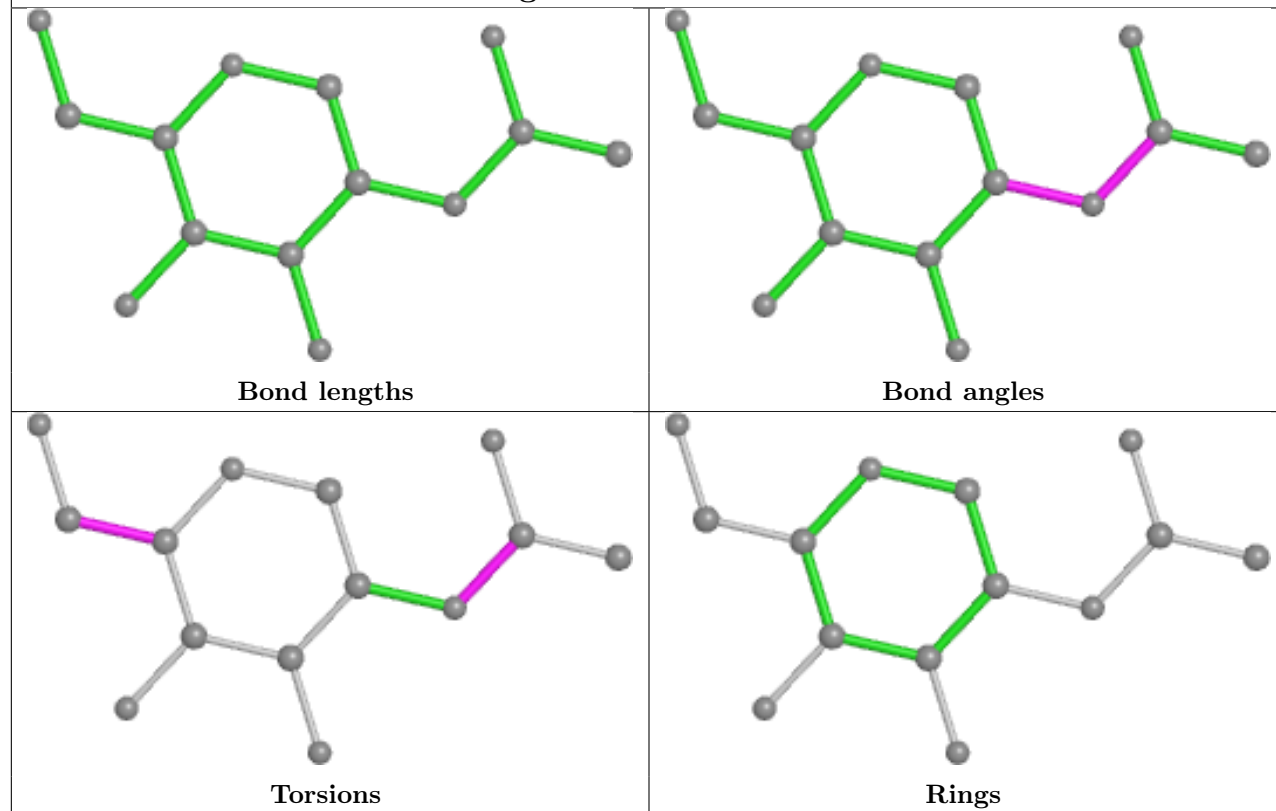




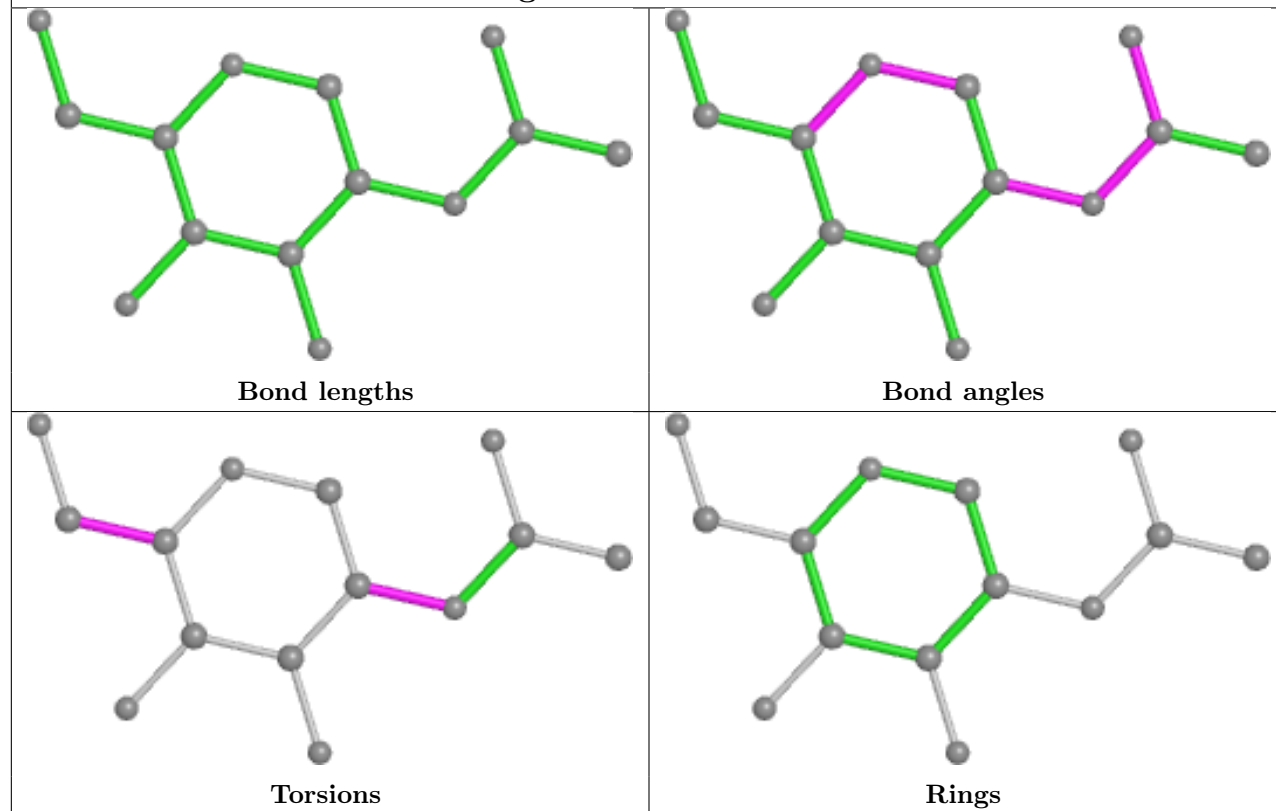




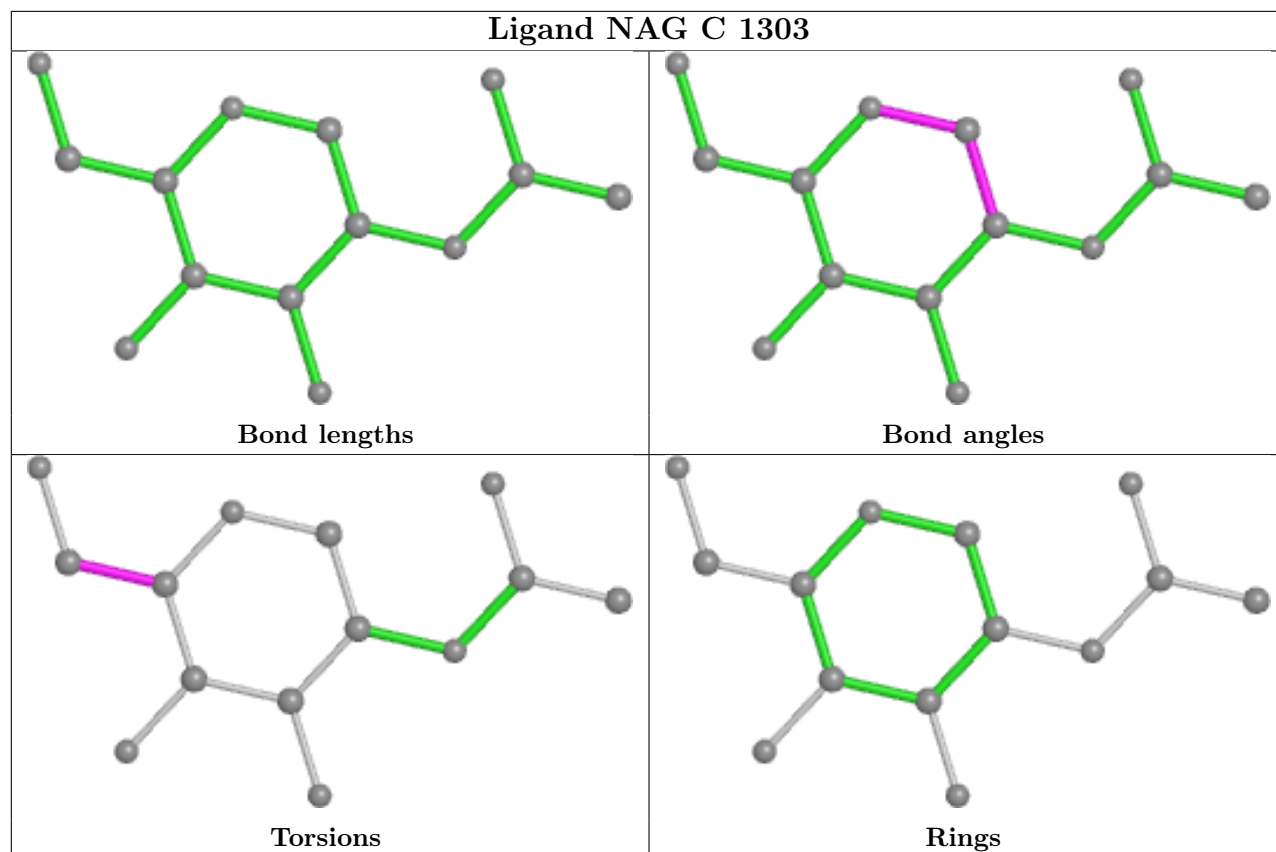
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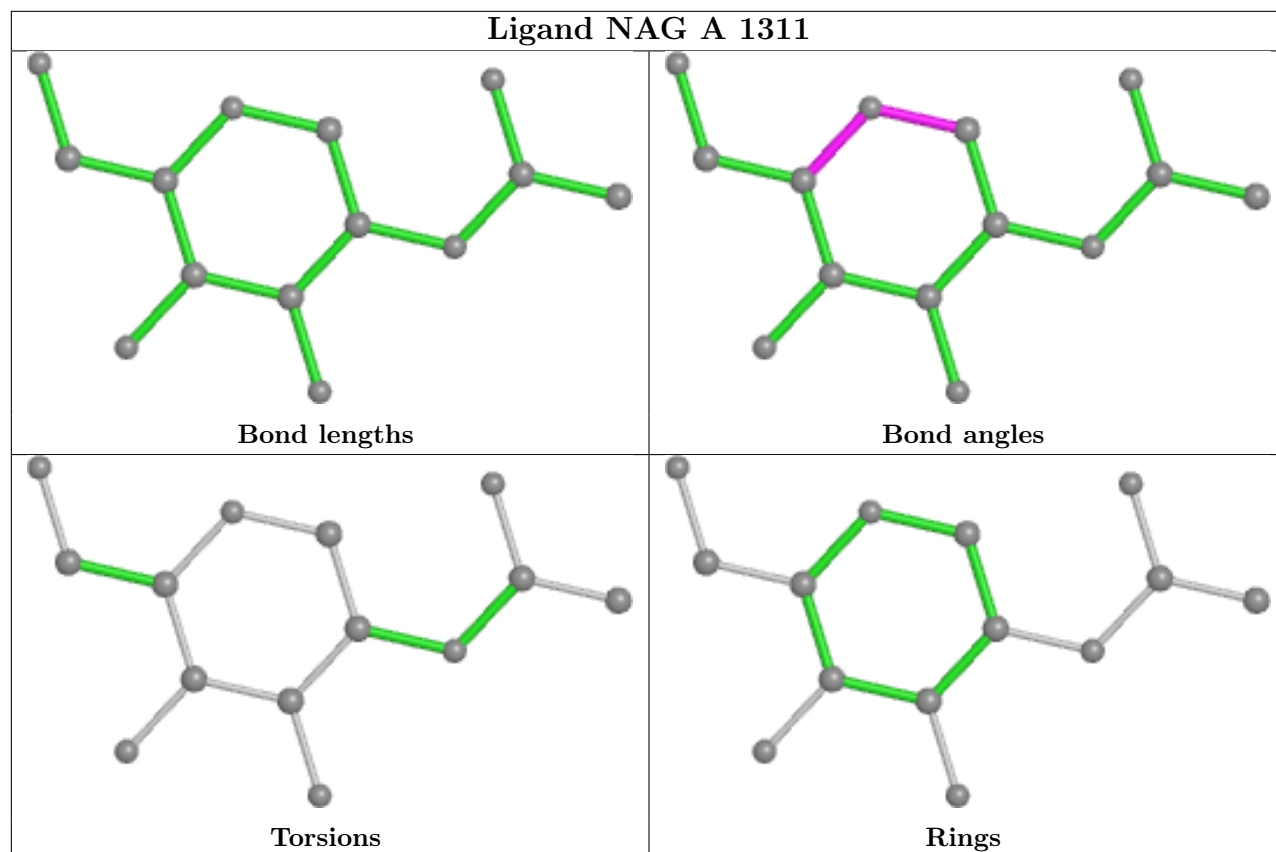
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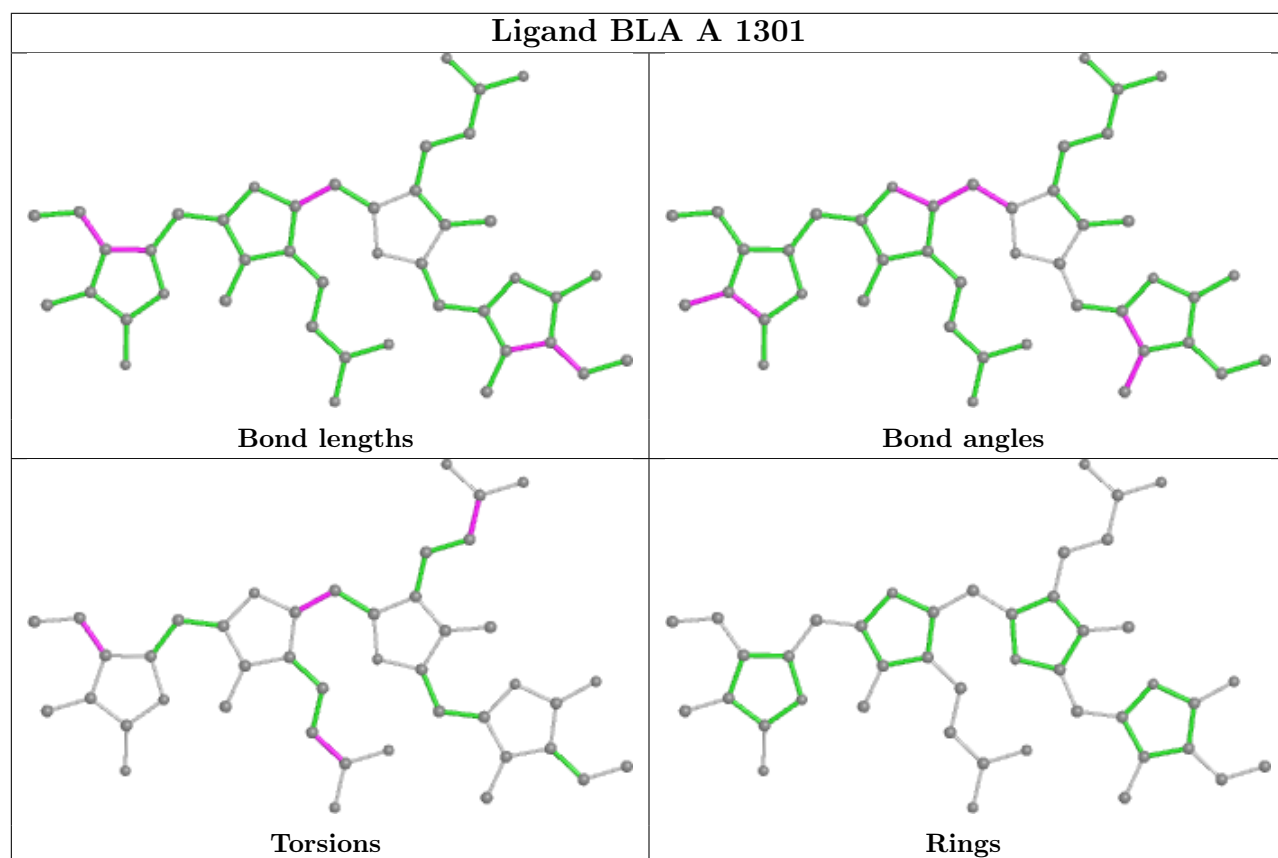
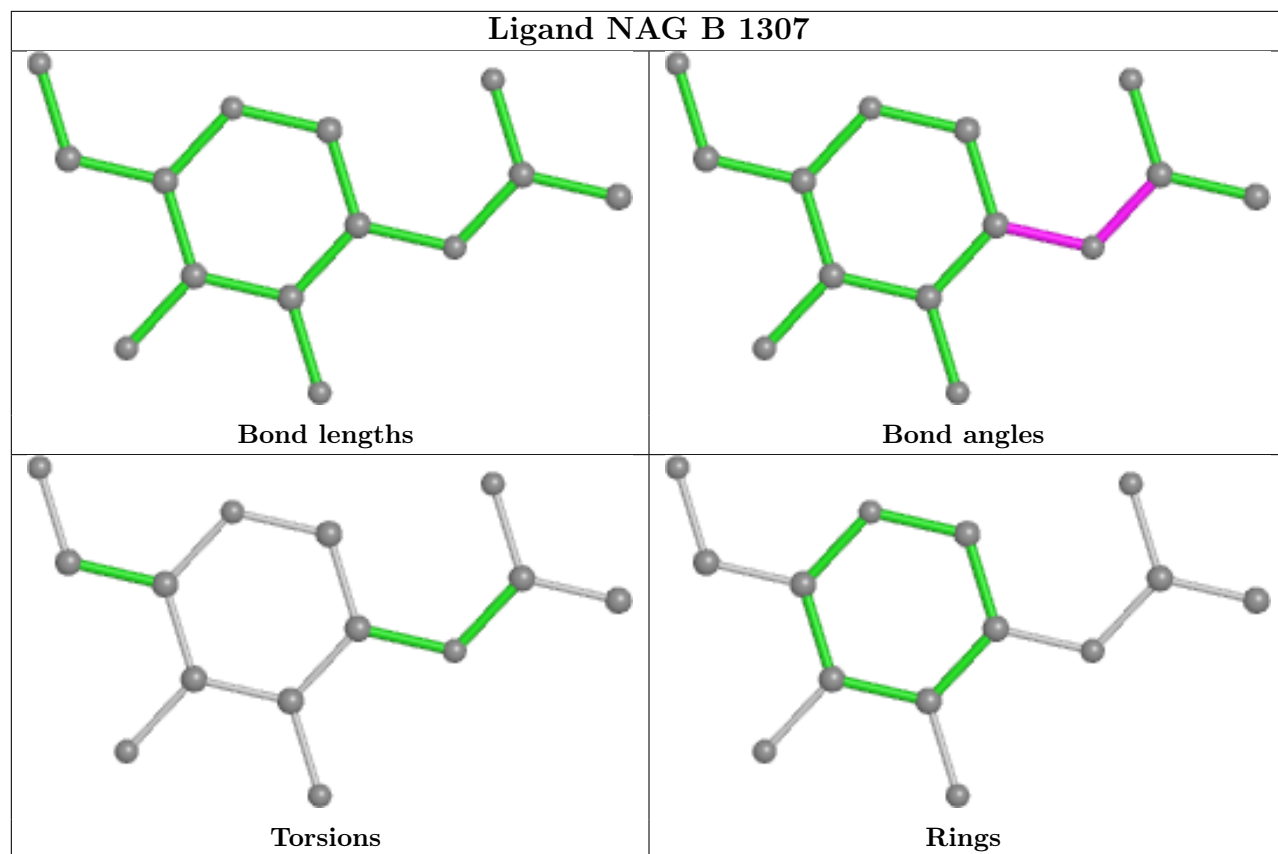


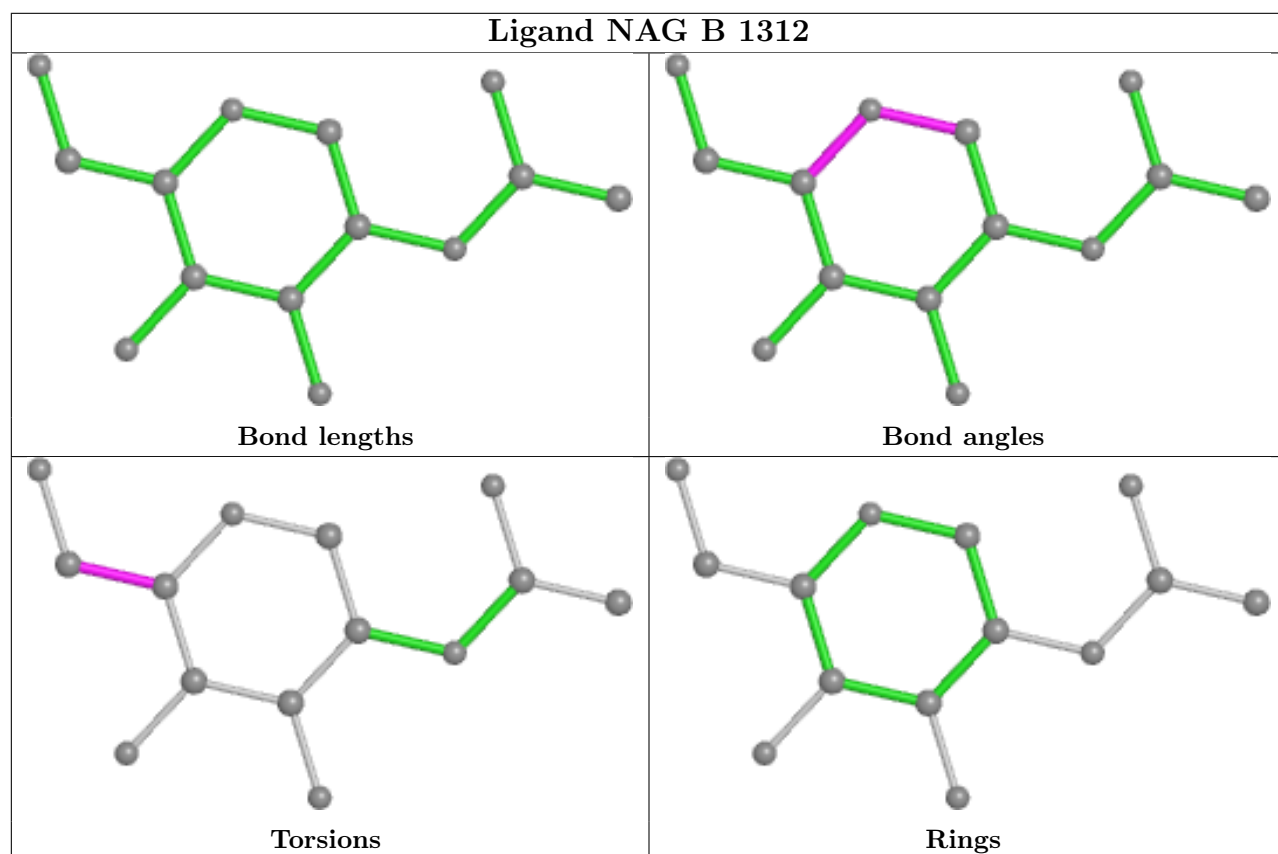
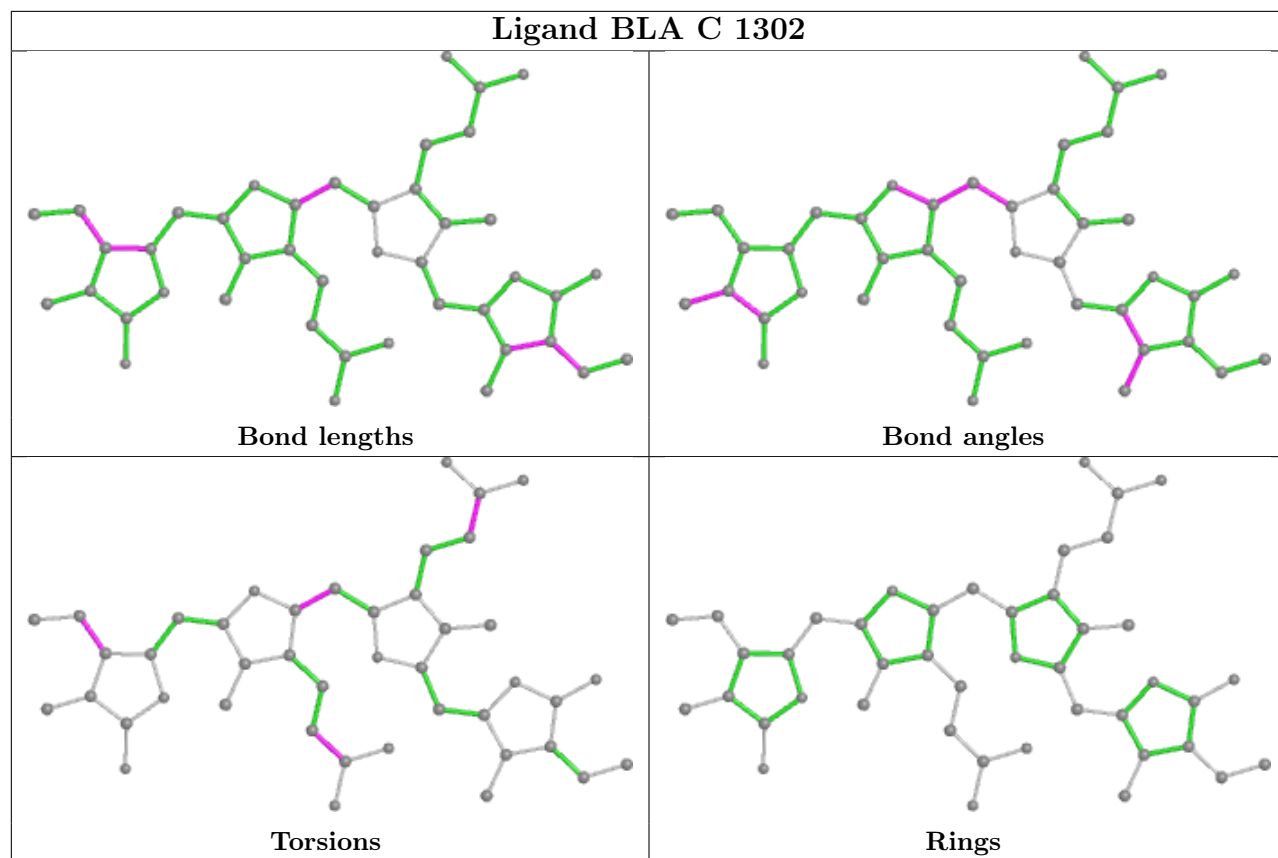
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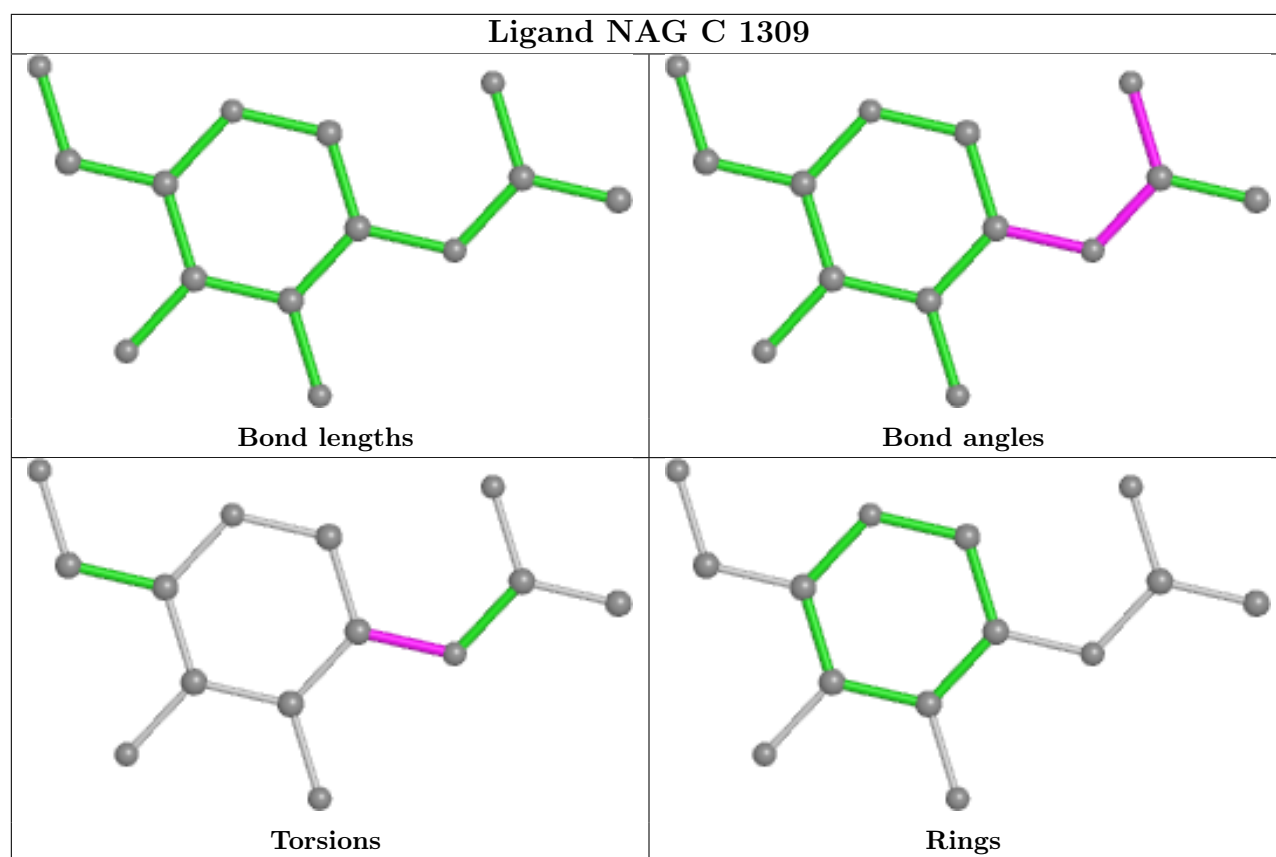


Ligand NAG A 1311









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.

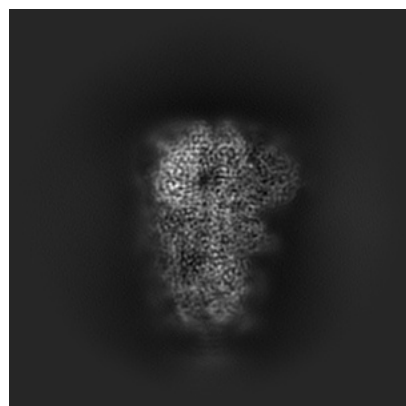
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65717. These allow visual inspection of the internal detail of the map and identification of artifacts.

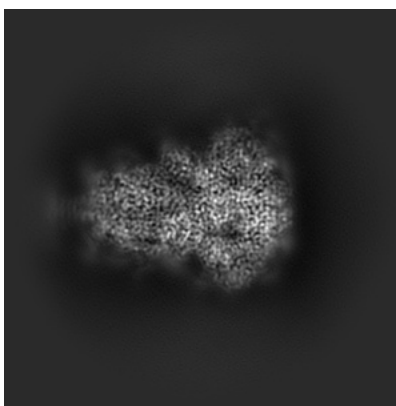
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

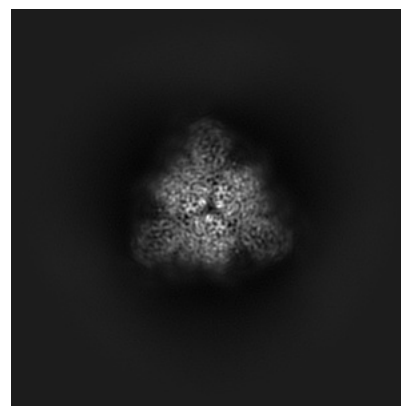
6.1.1 Primary map



X

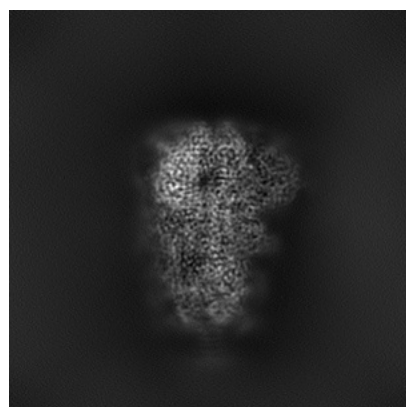


Y

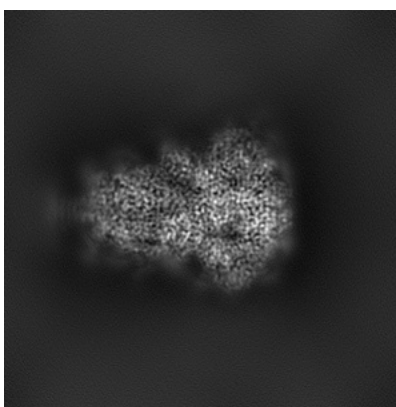


Z

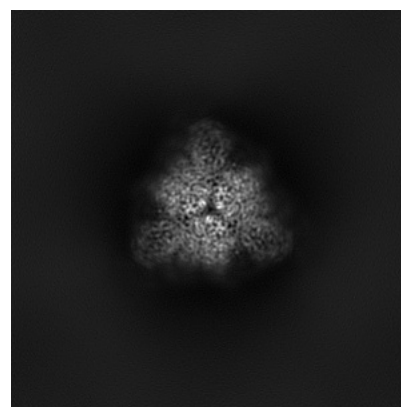
6.1.2 Raw map



X



Y

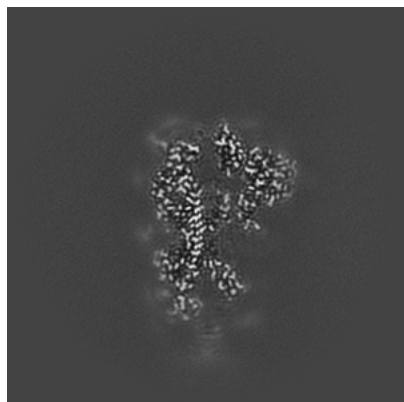


Z

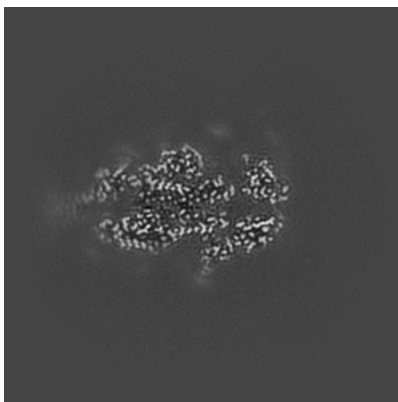
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

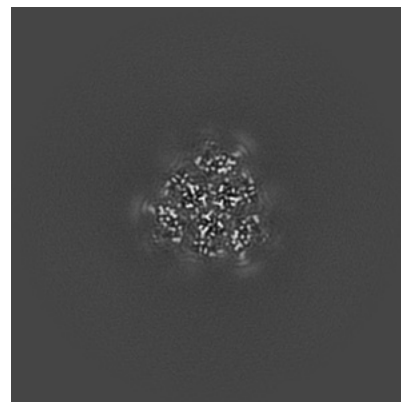
6.2.1 Primary map



X Index: 160

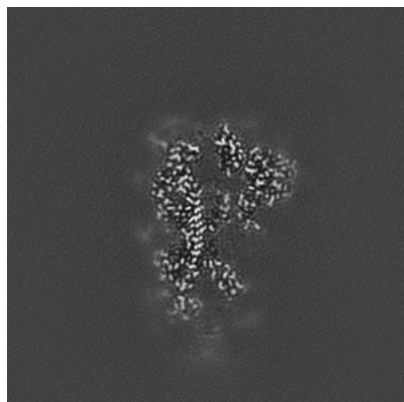


Y Index: 160

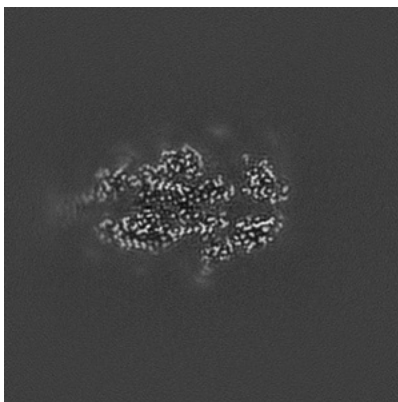


Z Index: 160

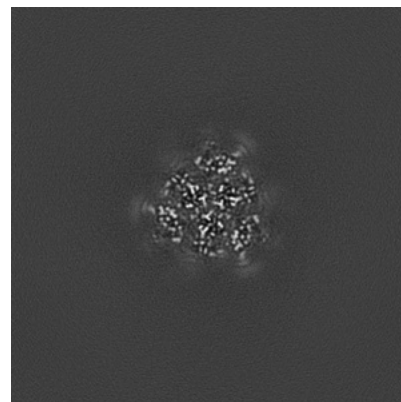
6.2.2 Raw map



X Index: 160



Y Index: 160

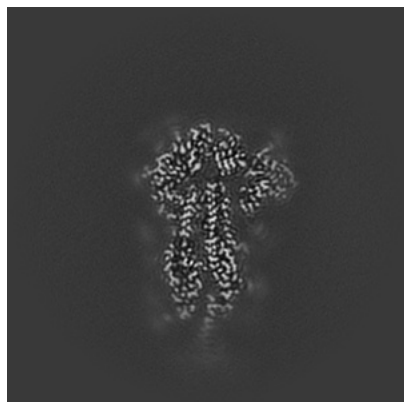


Z Index: 160

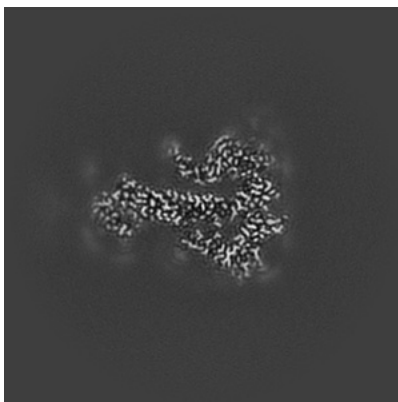
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

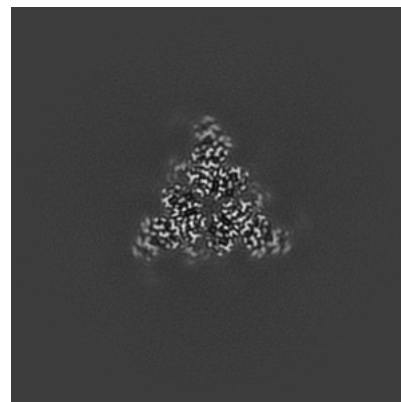
6.3.1 Primary map



X Index: 167

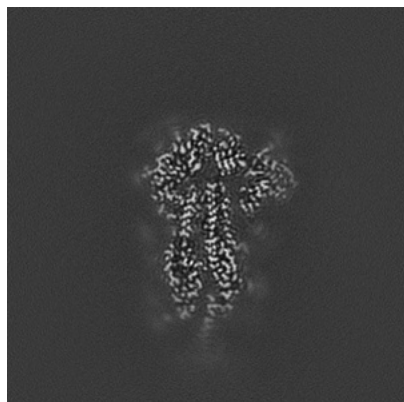


Y Index: 145

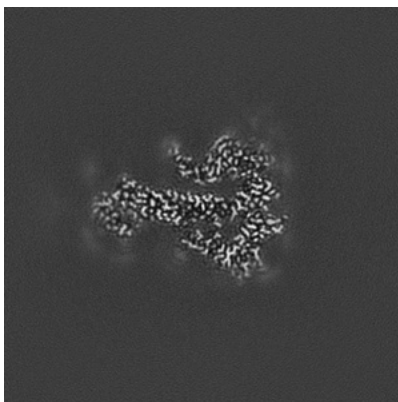


Z Index: 195

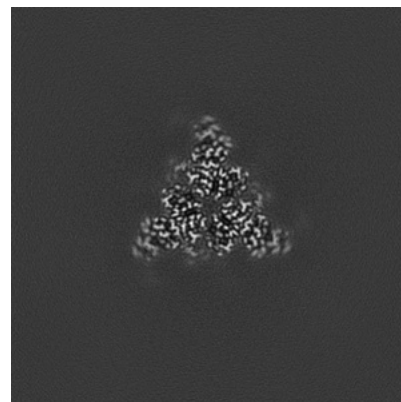
6.3.2 Raw map



X Index: 167



Y Index: 145

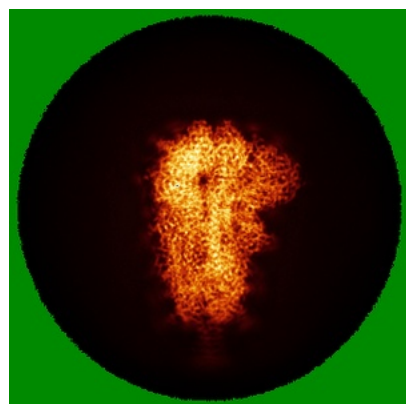


Z Index: 195

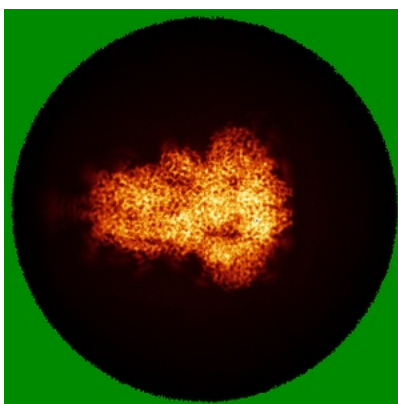
The images above show the largest variance slices of the map in three orthogonal directions.

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

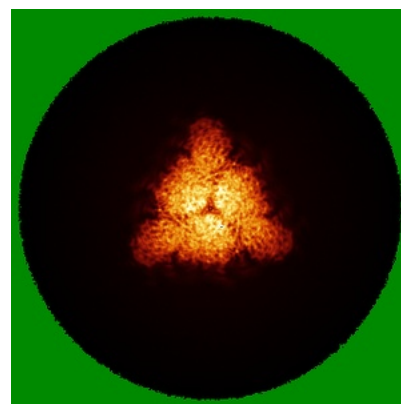
6.4.1 Primary map



X

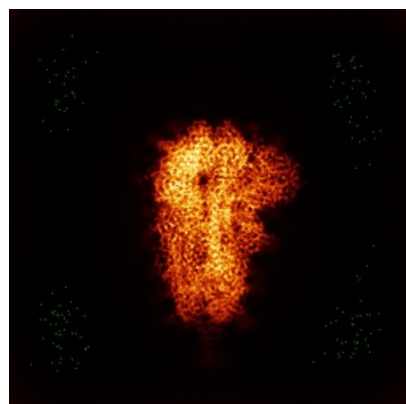


Y

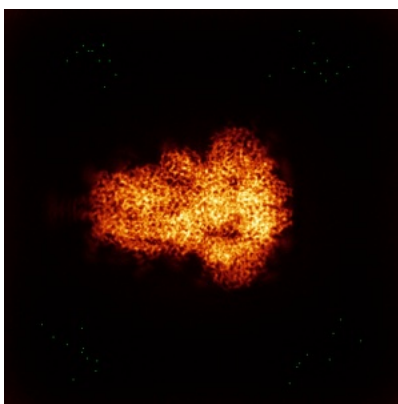


Z

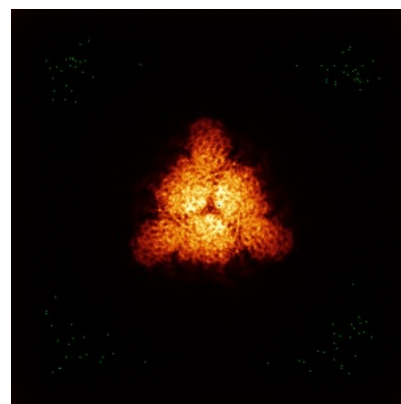
6.4.2 Raw map



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 0.08. 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.

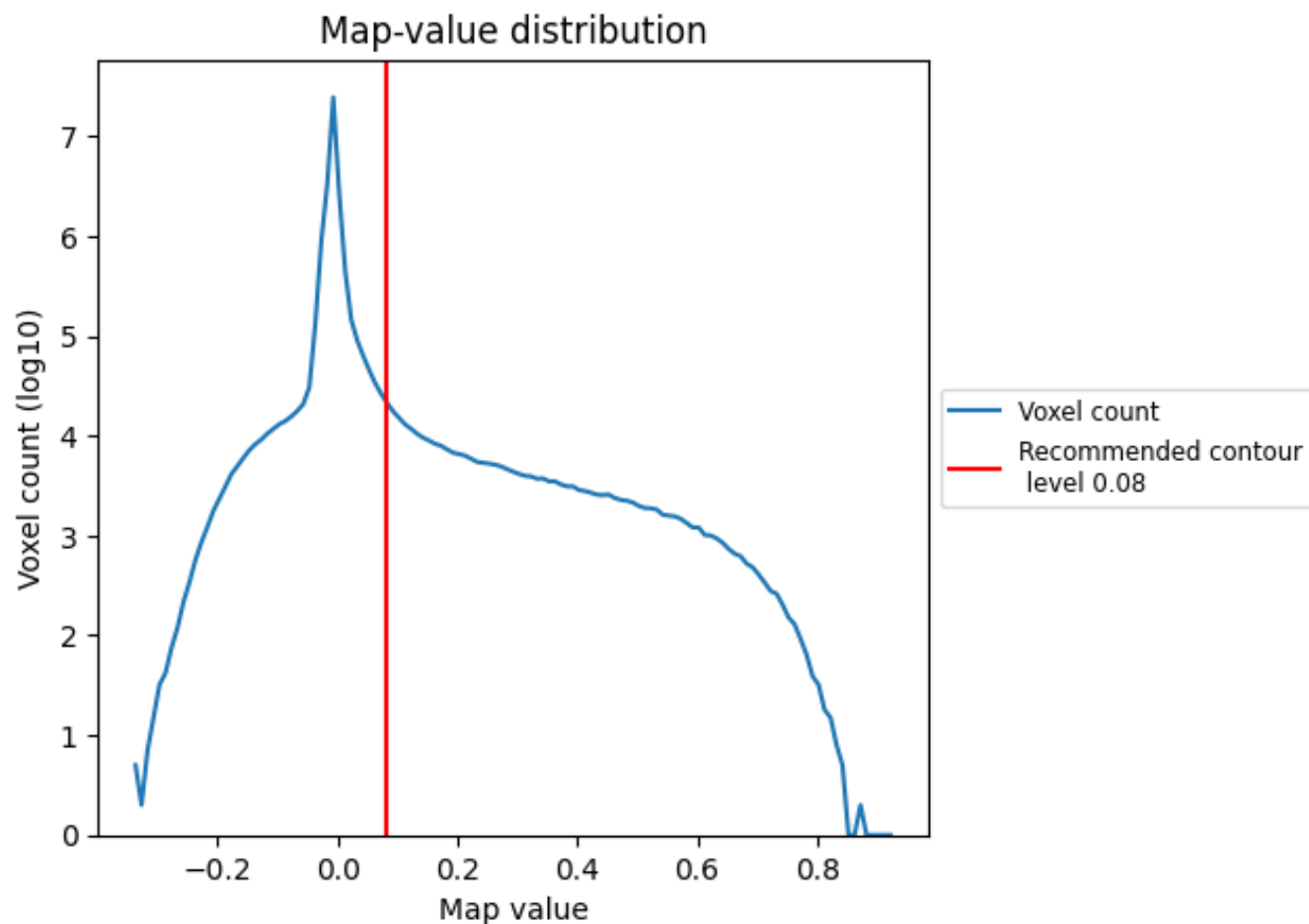
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

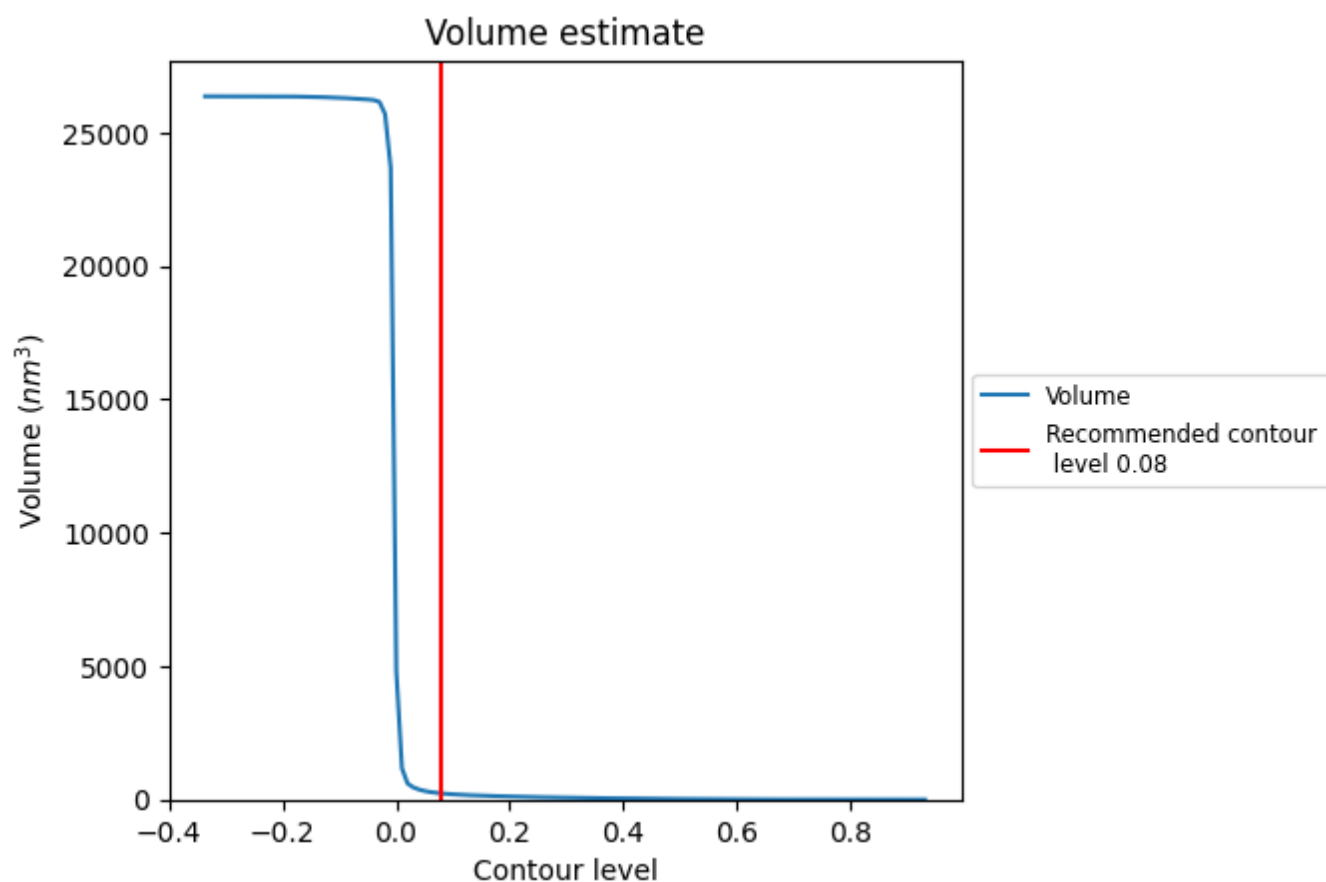
This section contains the results of statistical analysis of the map.

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.

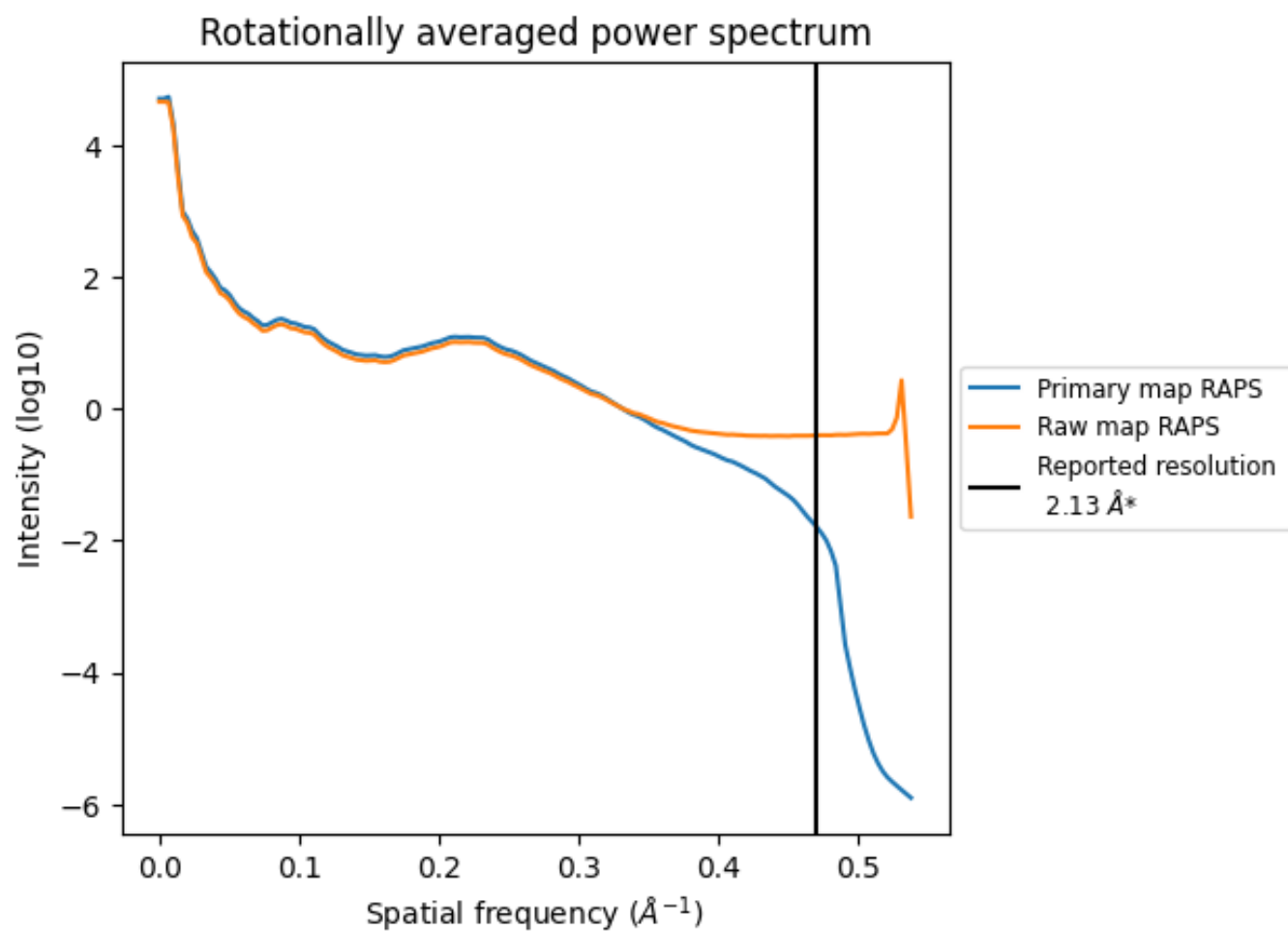
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 230 nm^3 ; this corresponds to an approximate mass of 208 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 ⓘ

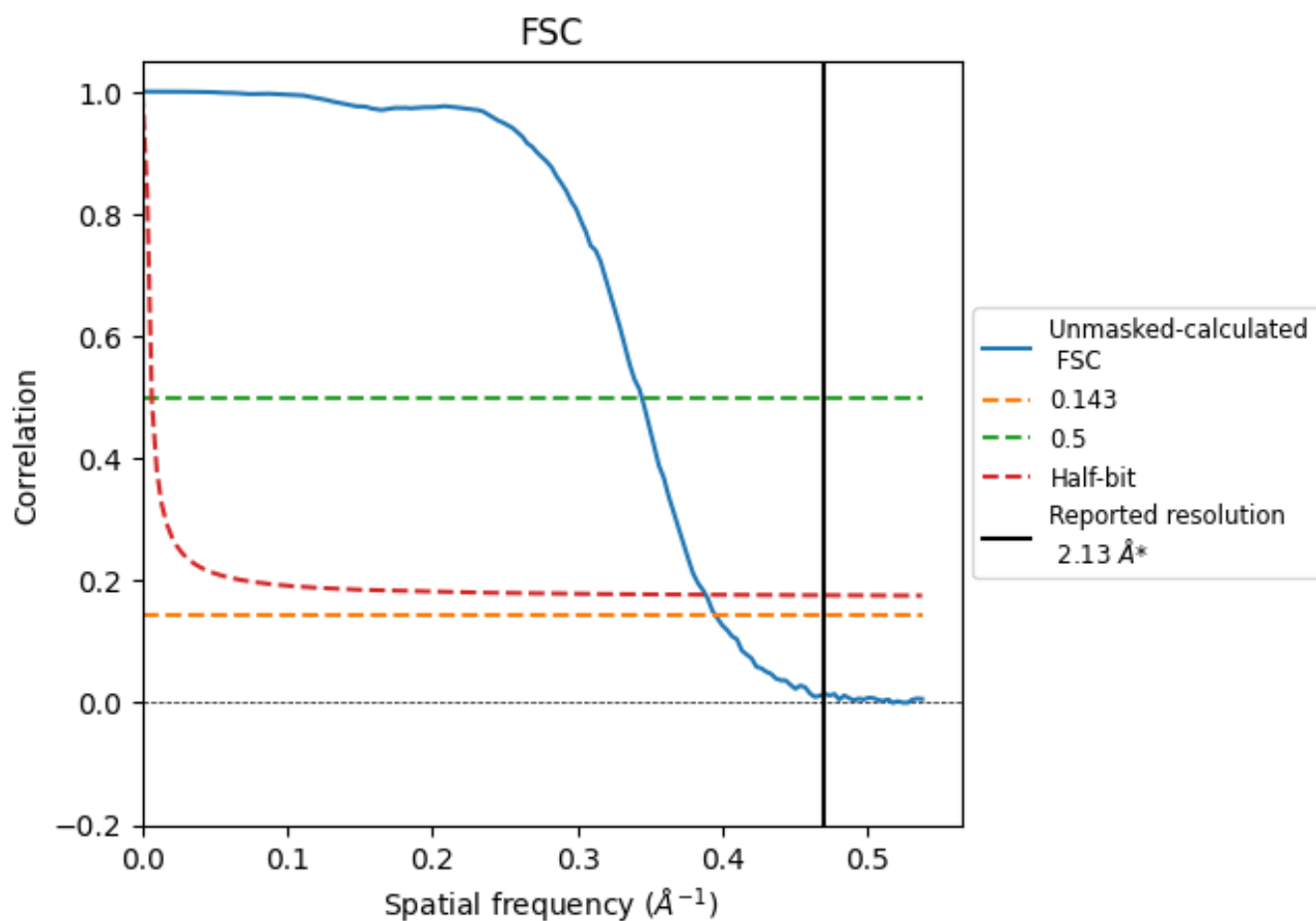


*Reported resolution corresponds to spatial frequency of 0.469 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.469 \AA^{-1}

8.2 Resolution estimates [i](#)

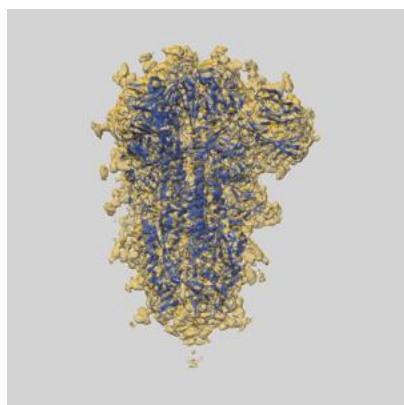
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.13	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.53	2.90	2.58

*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 2.53 differs from the reported value 2.13 by more than 10 %

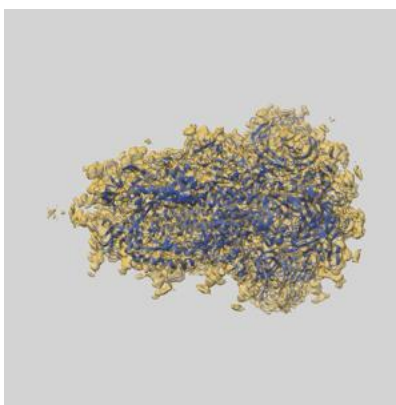
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65717 and PDB model 9W75. Per-residue inclusion information can be found in section [3](#) on page [10](#).

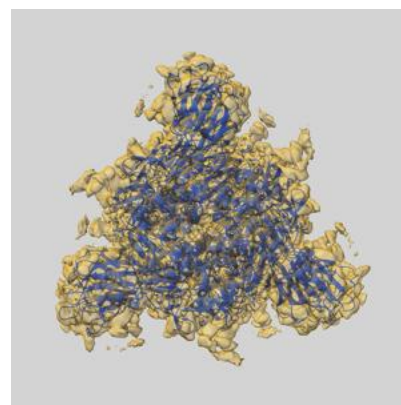
9.1 Map-model overlay [i](#)



X



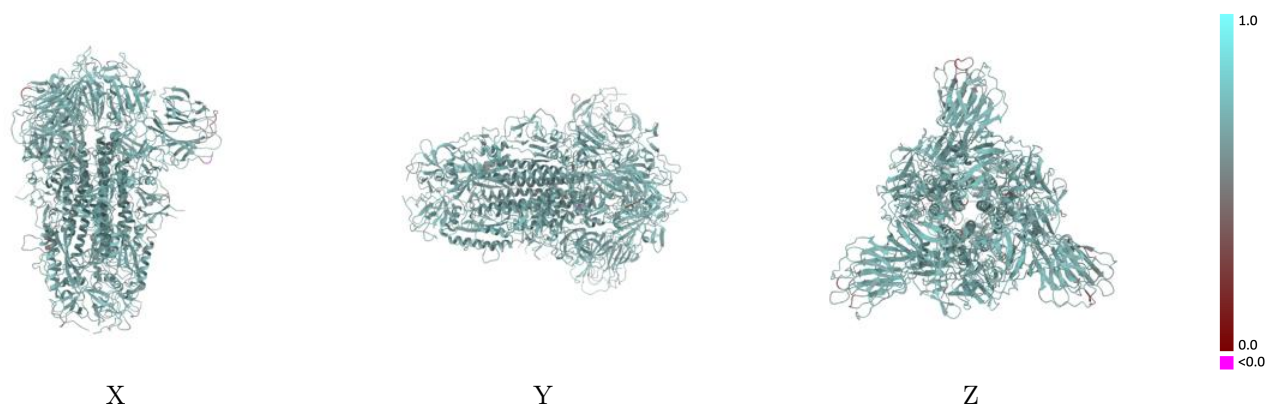
Y



Z

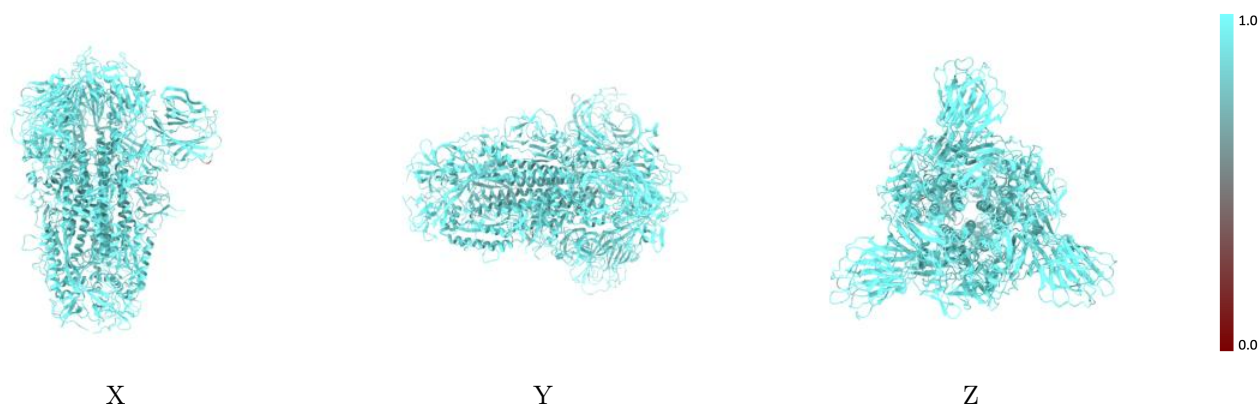
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



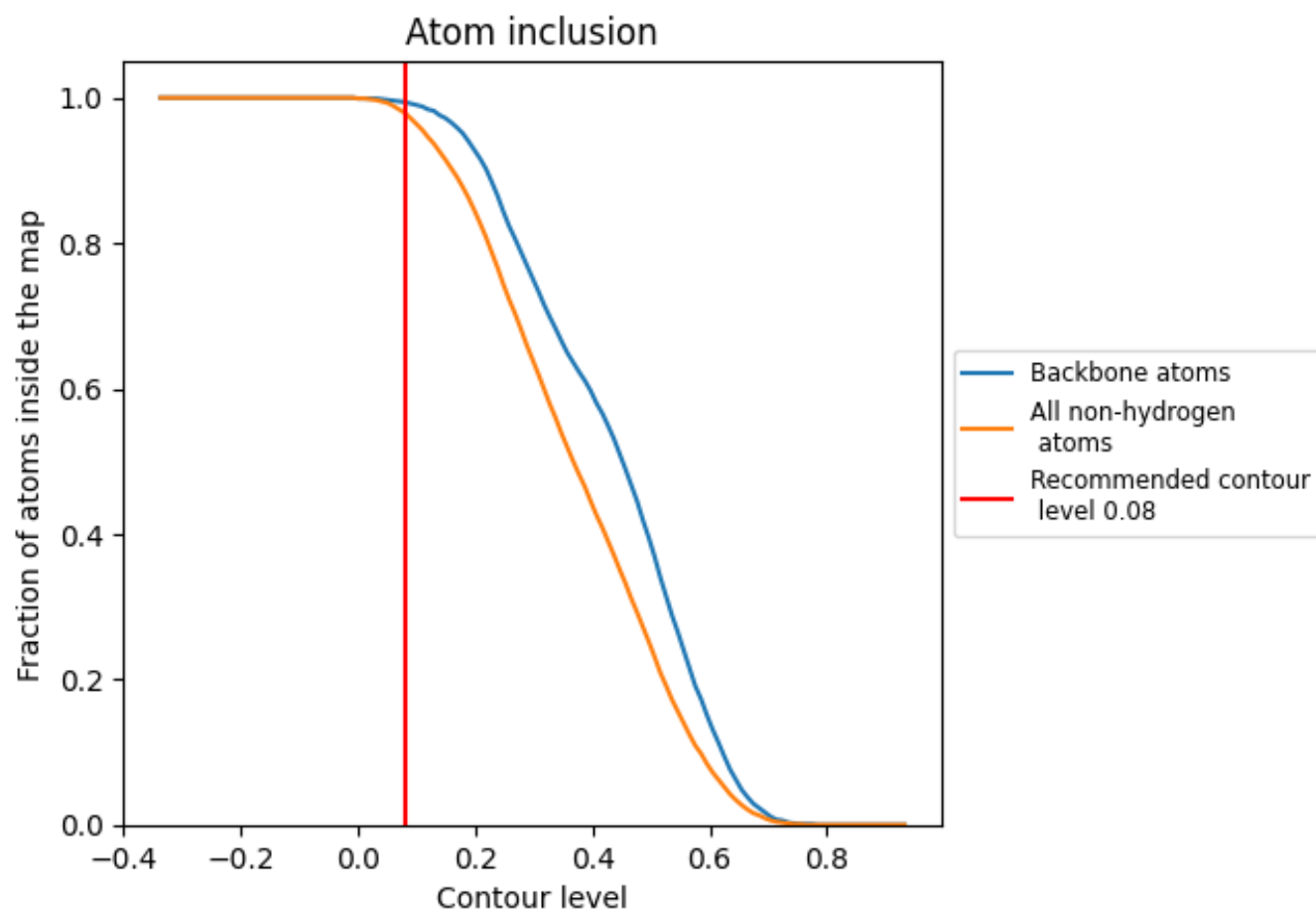
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9790	<div></div> 0.6410
A	<div></div> 0.9800	<div></div> 0.6410
B	<div></div> 0.9820	<div></div> 0.6480
C	<div></div> 0.9800	<div></div> 0.6420
D	<div></div> 1.0000	<div></div> 0.5690
E	<div></div> 0.8570	<div></div> 0.4630
F	<div></div> 1.0000	<div></div> 0.5960
G	<div></div> 0.9180	<div></div> 0.5650
H	<div></div> 0.9640	<div></div> 0.5480
I	<div></div> 0.8930	<div></div> 0.5030
J	<div></div> 0.8570	<div></div> 0.4660
K	<div></div> 0.7380	<div></div> 0.3320
L	<div></div> 0.9640	<div></div> 0.5850
M	<div></div> 0.9640	<div></div> 0.5480
N	<div></div> 0.7860	<div></div> 0.3860
O	<div></div> 0.9290	<div></div> 0.4800
P	<div></div> 0.9400	<div></div> 0.5760
Q	<div></div> 0.8210	<div></div> 0.4610

