



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:54 PM UTC

PDB ID : 8Y1H / pdb_00008y1h
EMDB ID : EMD-38836
Title : The 2up formation of the HKU1-B S protein in the apo state
Authors : Xia, L.Y.; Zhang, Y.Y.; Zhou, Q.
Deposited on : 2024-01-24
Resolution : 3.16 Å(reported)

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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:

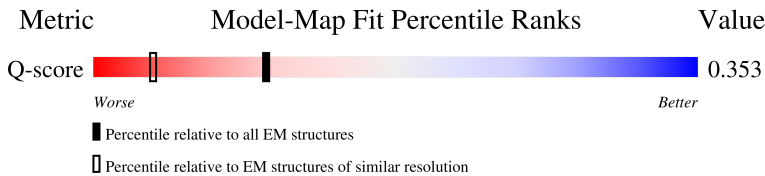
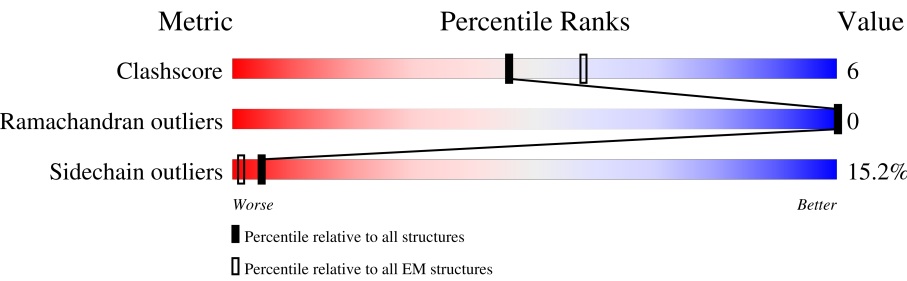
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.16 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	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14474 (2.66 - 3.66)

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	1290	12% 69% 22% 6%
1	B	1290	13% 69% 21% 6%
1	C	1290	68% 22% 6%
2	D	6	50% 33% 67%

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Mol	Chain	Length	Quality of chain
2	I	6	
2	N	6	
3	E	2	
3	F	2	
3	G	2	
3	H	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	

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.

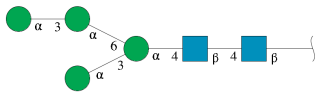
- Molecule 1 is a protein called Spike glycoprotein.

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

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- 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.



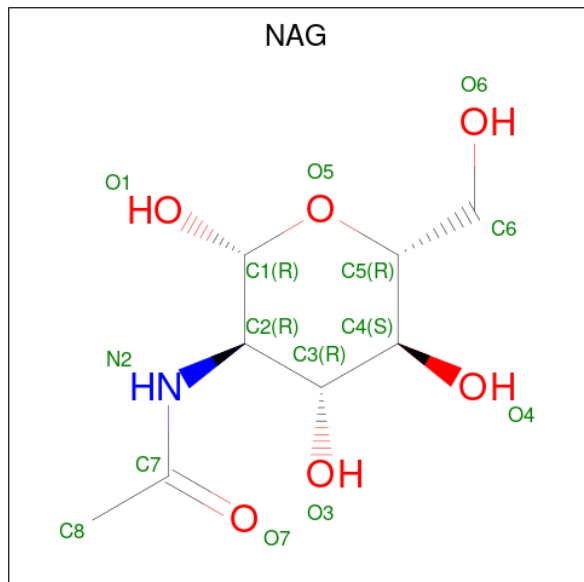
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	6	Total	C	N	O	0	0
			72	40	2	30		
2	I	6	Total	C	N	O	0	0
			72	40	2	30		
2	N	6	Total	C	N	O	0	0
			72	40	2	30		

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

- Molecule 4 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
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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

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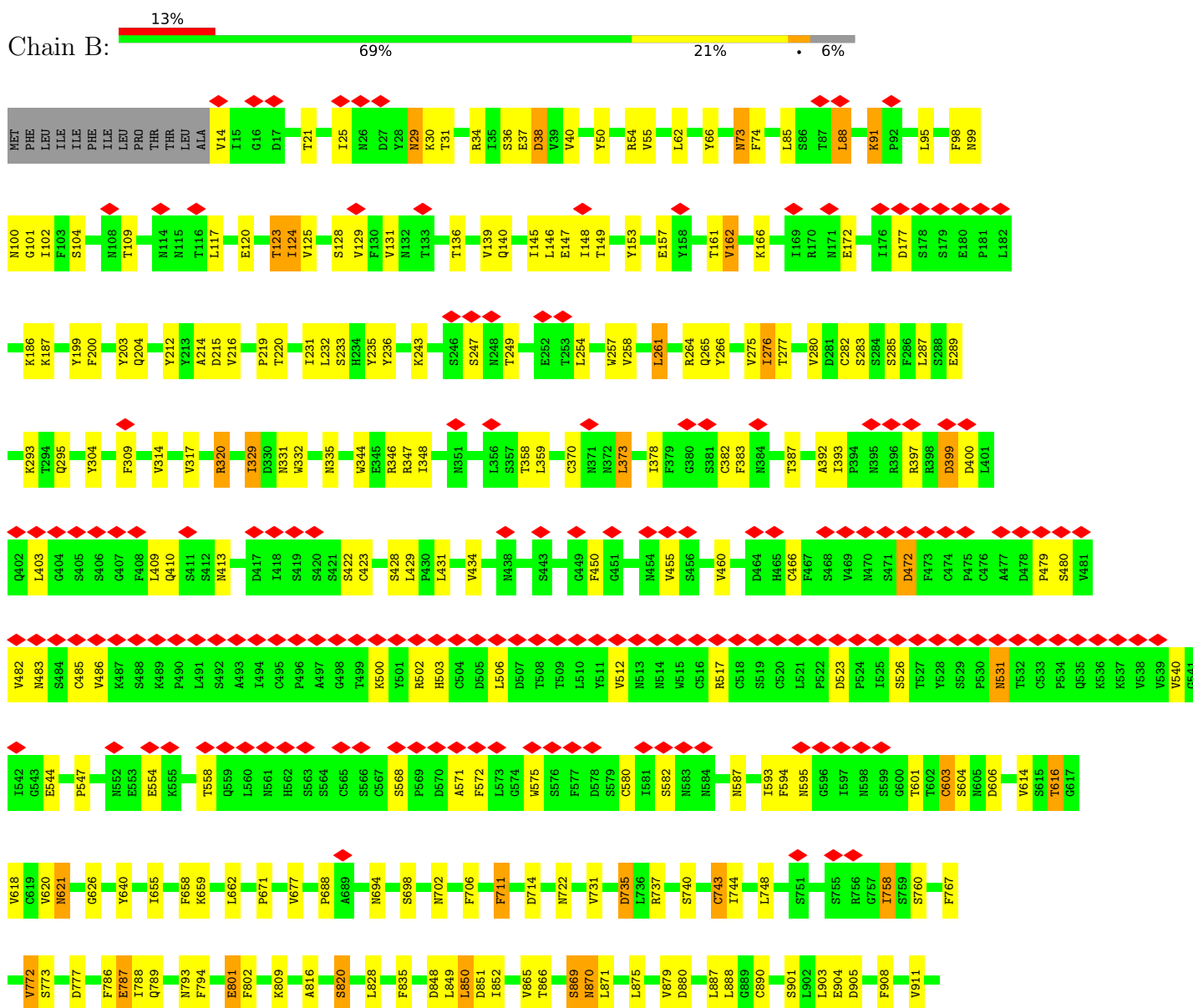
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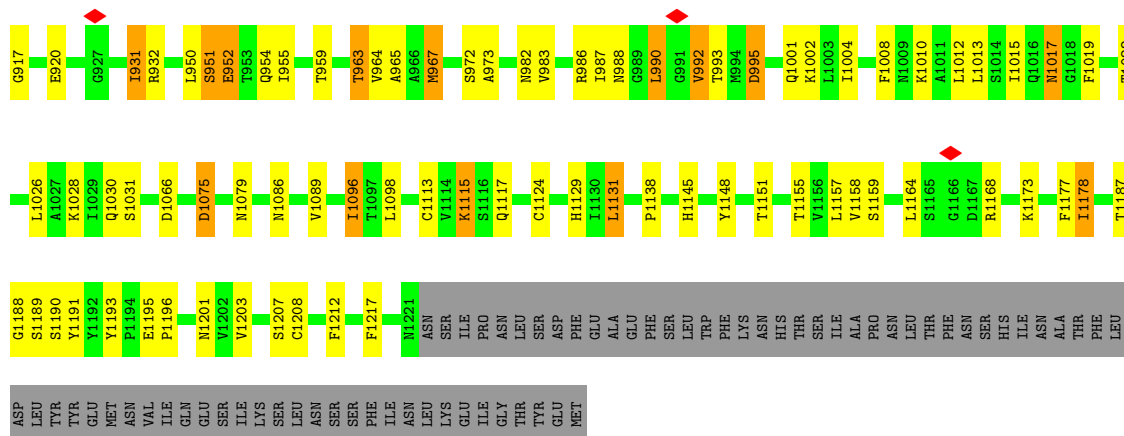
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4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

3 Residue-property plots

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.

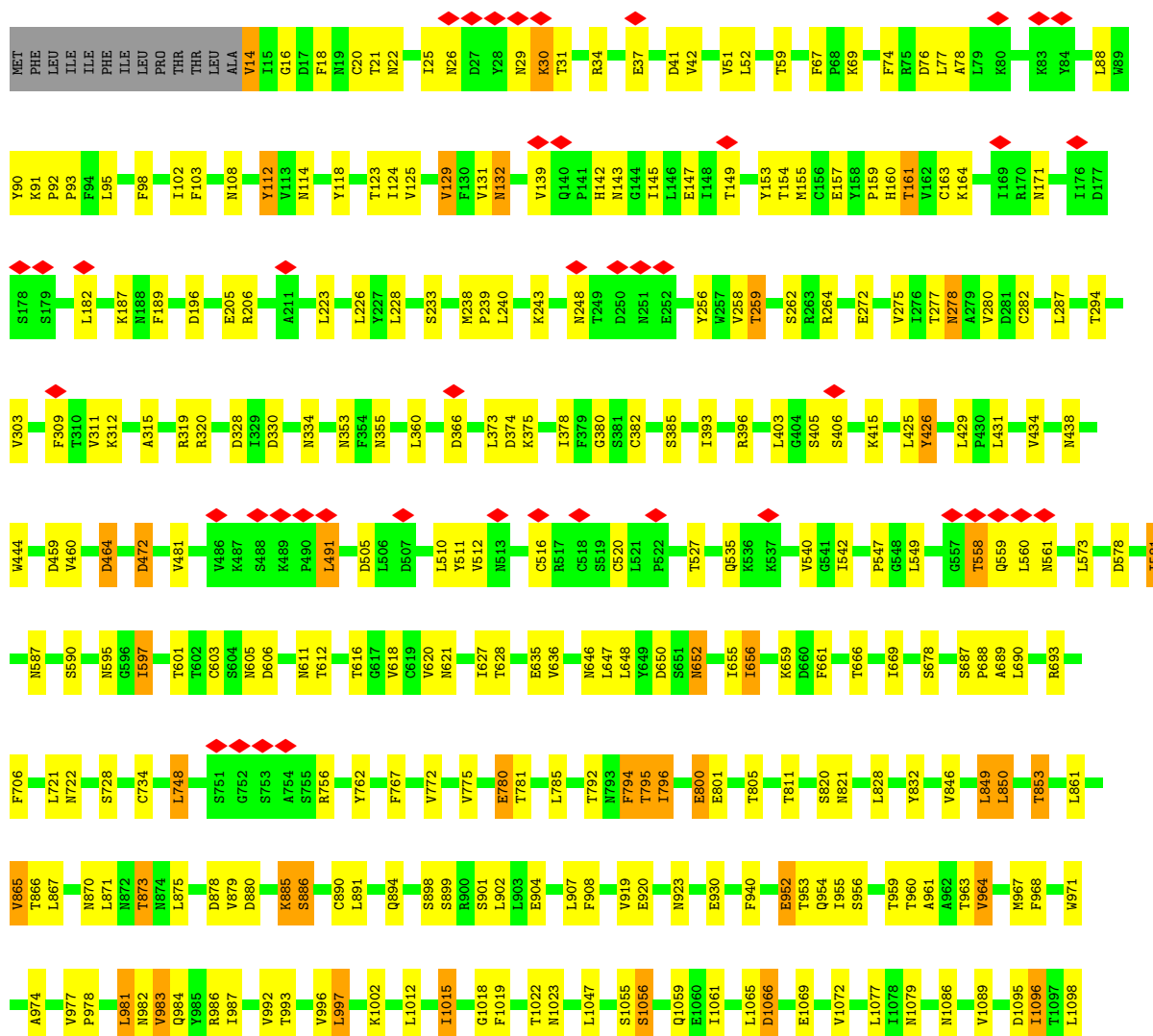
• Molecule 1: Spike glycoprotein

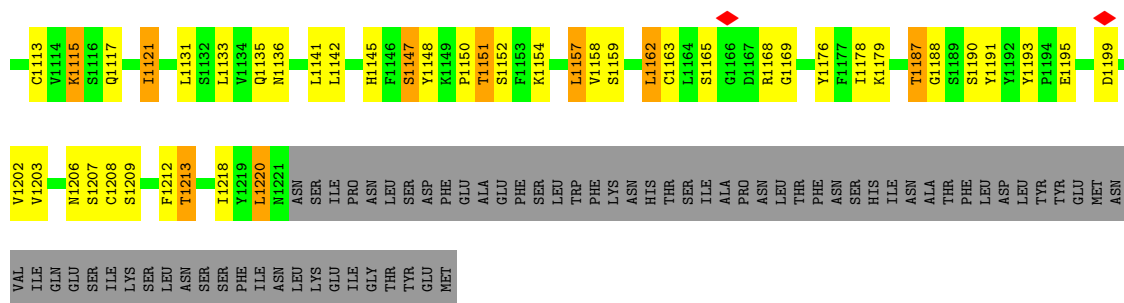




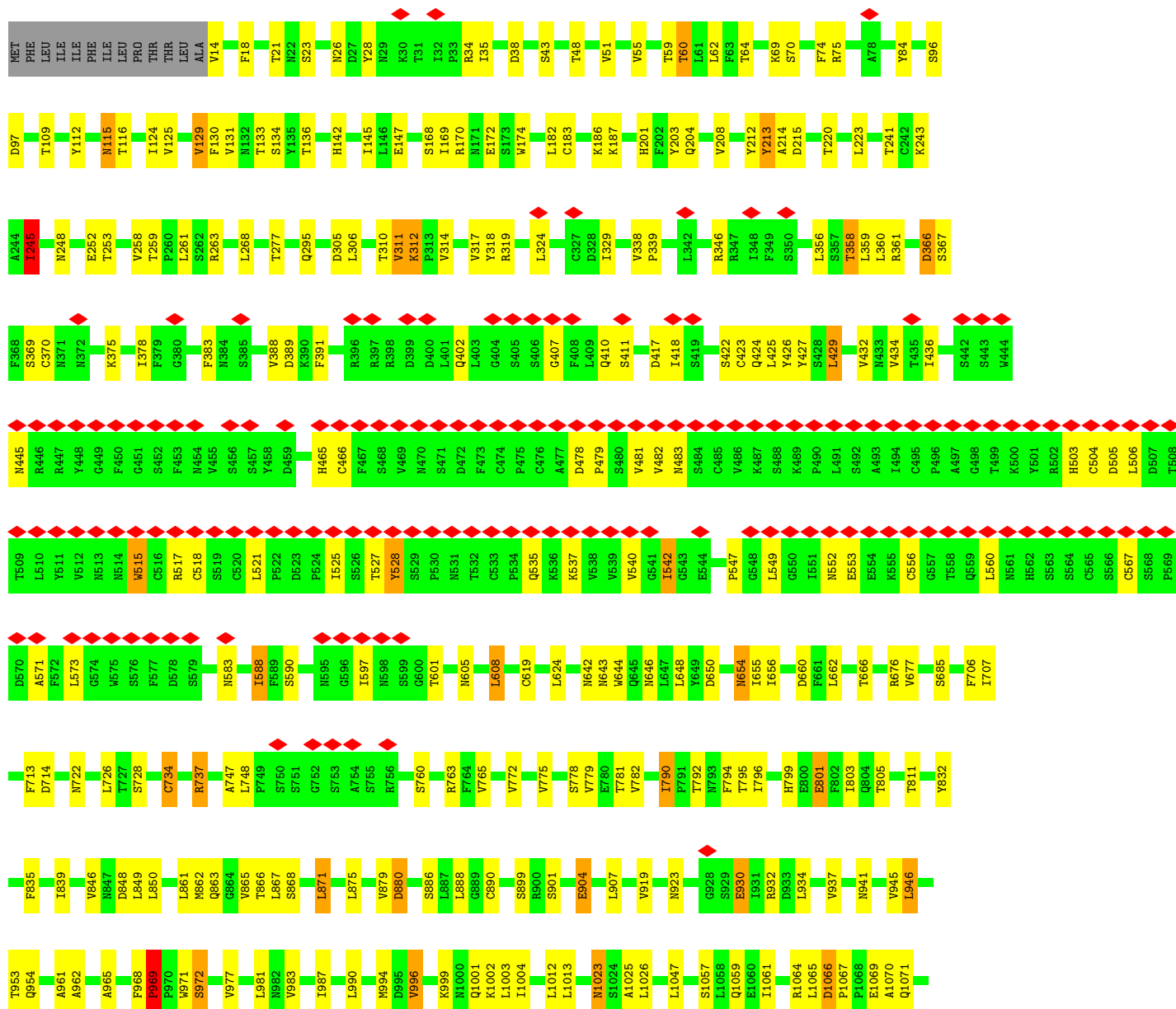
• Molecule 1: Spike glycoprotein

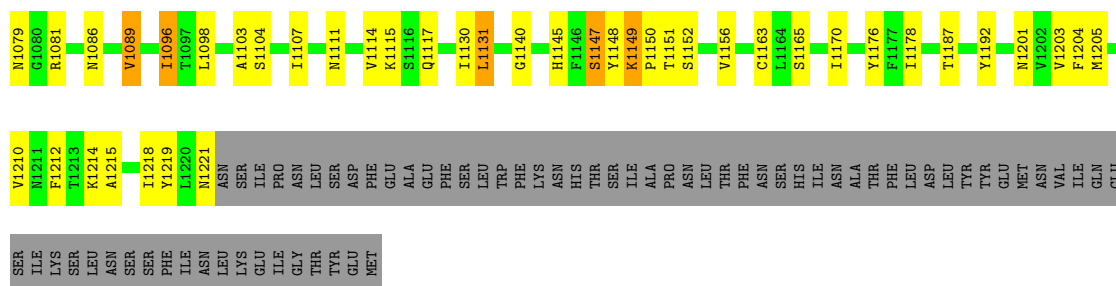
Chain C: 68% 22% 6%





• Molecule 1: Spike glycoprotein

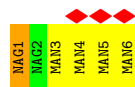




- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



- 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



- 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 G:



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

Chain H:



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

Chain J:



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

Chain K:



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

Chain L:



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

Chain M:



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

Chain O:  100%



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

Chain P:  50% 100%



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

Chain Q:  50% 50%



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

Chain R:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	134669	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	4.155	Depositor
Minimum map value	-2.881	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.33	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

5.1 Standard geometry

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

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	0.26	1/9653 (0.0%)	0.57	2/13146 (0.0%)
1	B	0.23	0/9653	0.55	3/13146 (0.0%)
1	C	0.26	0/9653	0.56	0/13146
All	All	0.25	1/28959 (0.0%)	0.56	5/39438 (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	4
1	C	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	945	VAL	C-N	-5.68	1.24	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ILE	N-CA-C	-6.74	106.73	113.20
1	B	329	ILE	N-CA-C	-6.54	107.12	113.53
1	A	969	PRO	N-CA-C	5.16	116.99	110.70
1	B	1148	TYR	CA-CB-CG	5.11	123.11	113.90
1	B	820	SER	N-CA-C	5.10	117.25	111.02

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	930	GLU	Peptide
1	A	968	PHE	Peptide
1	A	969	PRO	Peptide
1	A	972	SER	Peptide
1	C	968	PHE	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	9078	123	0
1	B	9425	0	9076	115	0
1	C	9425	0	9076	134	0
2	D	72	0	61	0	0
2	I	72	0	61	1	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	1	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	2	0
4	B	238	0	221	1	0
4	C	238	0	221	0	0
All	All	29541	0	28376	356	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 6.

All (356) 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:214:ALA:HB2	1:B:220:THR:HA	1.79	0.65
1:A:890:CYS:H	1:A:899:SER:HB2	1.61	0.65
1:C:690:LEU:HB2	1:C:721:LEU:HB2	1.79	0.64
1:C:315:ALA:H	1:C:620:VAL:HG12	1.61	0.64
1:C:801:GLU:OE1	1:C:1145:HIS:NE2	2.31	0.64
1:A:868:SER:HB3	1:A:871:LEU:HB2	1.81	0.63
1:C:353:ASN:HB3	1:C:605:ASN:HD22	1.63	0.63
1:C:287:LEU:HB3	1:C:688:PRO:HD3	1.82	0.61
1:A:201:HIS:HB3	1:A:212:TYR:HB2	1.82	0.61
1:C:795:THR:OG1	1:C:796:ILE:N	2.32	0.61
1:C:978:PRO:O	1:C:982:ASN:N	2.30	0.61
1:C:132:ASN:OD1	1:C:132:ASN:N	2.33	0.61
1:B:62:LEU:HD13	1:B:295:GLN:HG2	1.82	0.61
1:B:348:ILE:HG23	1:B:387:THR:HG22	1.83	0.60
1:A:429:LEU:HB2	1:A:588:ILE:HD11	1.84	0.60
1:B:904:GLU:O	1:B:908:PHE:HB2	2.02	0.60
1:A:366:ASP:N	1:A:366:ASP:OD1	2.34	0.60
1:B:466:CYS:HB3	1:B:547:PRO:HD2	1.84	0.59
1:C:971:TRP:HB3	1:C:974:ALA:HB3	1.85	0.59
1:A:183:CYS:SG	1:A:186:LYS:NZ	2.76	0.58
1:C:650:ASP:HB3	1:C:656:ILE:HD11	1.84	0.58
1:A:504:CYS:HA	1:A:518:CYS:HA	1.85	0.58
1:A:518:CYS:HB2	1:A:521:LEU:HD21	1.86	0.58
1:A:1023:ASN:HD22	1:A:1025:ALA:H	1.51	0.58
1:C:92:PRO:HA	1:C:95:LEU:HB3	1.86	0.58
1:C:627:ILE:HG21	1:C:655:ILE:HD13	1.86	0.57
1:C:1165:SER:O	1:C:1168:ARG:NH2	2.37	0.57
1:A:370:CYS:HA	1:A:423:CYS:HA	1.86	0.57
1:B:793:ASN:HB3	1:B:1151:THR:HB	1.85	0.57
1:A:338:VAL:HG21	1:A:434:VAL:HG13	1.87	0.57
1:B:735:ASP:OD1	1:B:735:ASP:N	2.37	0.57
1:B:1013:LEU:O	1:B:1017:ASN:ND2	2.38	0.57
1:B:293:LYS:HE3	1:B:304:TYR:HB3	1.88	0.56
1:A:23:SER:O	1:A:170:ARG:NH1	2.39	0.56
1:B:344:TRP:NE1	1:B:413:ASN:O	2.39	0.56
1:C:920:GLU:HA	1:C:923:ASN:HD22	1.71	0.56
1:B:606:ASP:HA	3:G:1:NAG:H82	1.87	0.56
1:C:319:ARG:NH1	1:C:612:THR:O	2.38	0.56
1:C:772:VAL:HG21	1:A:867:LEU:HB2	1.86	0.56
1:B:472:ASP:N	1:B:472:ASP:OD1	2.38	0.56
1:B:1075:ASP:O	1:B:1079:ASN:ND2	2.39	0.56
1:A:832:TYR:OH	1:A:1079:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ASP:OD1	1:C:472:ASP:N	2.39	0.55
1:C:901:SER:OG	1:C:902:LEU:N	2.38	0.55
1:B:162:VAL:HB	1:B:172:GLU:HB2	1.89	0.55
1:B:973:ALA:HB2	1:B:1115:LYS:HE2	1.89	0.55
1:A:713:PHE:HB2	4:A:2012:NAG:H82	1.89	0.55
1:B:370:CYS:HA	1:B:423:CYS:HA	1.88	0.55
1:C:67:PHE:O	1:C:264:ARG:NH1	2.40	0.55
1:C:88:LEU:HA	1:C:91:LYS:HD3	1.87	0.55
1:C:103:PHE:HB3	1:C:259:THR:HG23	1.89	0.55
1:C:425:LEU:HB3	1:C:590:SER:HB3	1.88	0.55
1:C:1055:SER:OG	1:C:1056:SER:N	2.40	0.55
1:A:747:ALA:HB2	1:A:763:ARG:HH21	1.72	0.55
1:C:846:VAL:HG13	1:C:1096:ILE:HG13	1.89	0.55
1:A:919:VAL:O	1:A:923:ASN:ND2	2.39	0.55
1:C:767:PHE:O	1:A:954:GLN:NE2	2.39	0.54
1:B:694:ASN:HD21	1:C:919:VAL:HG13	1.72	0.54
4:B:2014:NAG:O7	1:C:870:ASN:ND2	2.41	0.54
1:C:886:SER:O	1:C:901:SER:OG	2.22	0.54
1:B:104:SER:HB2	1:B:200:PHE:HB2	1.89	0.54
1:A:213:TYR:HB3	1:A:223:LEU:HD22	1.90	0.54
1:B:123:THR:OG1	1:B:124:ILE:N	2.40	0.54
1:C:320:ARG:O	1:C:611:ASN:ND2	2.40	0.54
1:A:425:LEU:HB3	1:A:590:SER:HB3	1.89	0.54
1:B:314:VAL:HB	1:B:620:VAL:HG12	1.90	0.54
1:A:402:GLN:O	1:A:410:GLN:NE2	2.41	0.54
1:A:478:ASP:HB3	1:A:481:VAL:HG22	1.90	0.54
1:B:967:MET:SD	1:B:967:MET:N	2.78	0.53
1:C:794:PHE:HA	1:C:1150:PRO:HA	1.91	0.53
1:C:628:THR:OG1	1:A:1059:GLN:NE2	2.41	0.53
1:B:88:LEU:HA	1:B:91:LYS:HD3	1.91	0.53
1:C:14:VAL:N	1:C:157:GLU:OE1	2.41	0.53
1:A:479:PRO:O	1:A:483:ASN:ND2	2.41	0.53
1:C:959:THR:O	1:C:963:THR:OG1	2.24	0.53
1:A:339:PRO:HG2	1:A:391:PHE:HA	1.90	0.53
1:A:801:GLU:OE2	1:A:1145:HIS:NE2	2.36	0.53
1:B:397:ARG:HD3	1:B:409:LEU:HG	1.90	0.53
1:B:901:SER:H	1:B:904:GLU:HB2	1.74	0.53
1:B:1187:THR:OG1	1:B:1188:GLY:N	2.42	0.53
1:B:995:ASP:N	1:B:995:ASP:OD1	2.39	0.52
1:C:278:ASN:OD1	1:C:278:ASN:N	2.41	0.52
1:C:650:ASP:OD2	1:C:652:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:VAL:O	1:A:312:LYS:NZ	2.43	0.52
1:A:425:LEU:HG	1:A:427:TYR:HB3	1.91	0.52
1:C:382:CYS:HA	1:C:603:CYS:HA	1.91	0.52
1:B:147:GLU:OE2	1:B:186:LYS:NZ	2.42	0.52
1:B:422:SER:HA	1:B:593:ILE:HA	1.91	0.52
1:A:1147:SER:OG	1:A:1148:TYR:N	2.41	0.52
1:C:78:ALA:HB2	1:C:256:TYR:HB2	1.92	0.52
1:A:734:CYS:O	1:A:737:ARG:NH1	2.37	0.52
1:B:347:ARG:NH2	3:F:1:NAG:O6	2.43	0.52
1:C:1187:THR:OG1	1:C:1188:GLY:N	2.42	0.52
1:A:650:ASP:OD1	1:A:650:ASP:N	2.43	0.52
1:C:129:VAL:HB	1:C:131:VAL:HG22	1.92	0.52
1:B:382:CYS:HA	1:B:603:CYS:HA	1.90	0.52
1:C:160:HIS:NE2	1:C:171:ASN:O	2.43	0.52
1:B:399:ASP:N	1:B:399:ASP:OD1	2.41	0.51
1:B:911:VAL:HG21	1:B:1138:PRO:HG2	1.91	0.51
1:A:886:SER:O	1:A:901:SER:OG	2.28	0.51
1:B:1164:LEU:HB2	1:B:1168:ARG:HB2	1.92	0.51
1:A:996:VAL:HA	1:A:999:LYS:HB2	1.92	0.51
1:C:124:ILE:HG22	1:C:139:VAL:HB	1.93	0.51
1:B:621:ASN:HD21	1:C:1059:GLN:HE22	1.56	0.51
1:C:656:ILE:O	1:C:669:ILE:N	2.39	0.51
1:C:678:SER:OG	1:C:693:ARG:NH2	2.43	0.51
1:C:1162:LEU:HD12	1:C:1213:THR:HB	1.92	0.51
1:B:373:LEU:HD11	1:B:594:PHE:HB2	1.93	0.51
1:C:1151:THR:OG1	1:C:1152:SER:N	2.43	0.51
1:A:535:GLN:NE2	1:A:553:GLU:OE2	2.43	0.51
1:C:98:PHE:HE2	1:C:102:ILE:HG12	1.75	0.51
1:C:142:HIS:HB2	1:C:145:ILE:HB	1.92	0.51
1:C:1066:ASP:OD1	1:C:1066:ASP:N	2.41	0.51
1:B:965:ALA:O	1:B:972:SER:N	2.43	0.51
1:A:23:SER:OG	1:A:170:ARG:NH1	2.44	0.51
1:A:805:THR:H	1:A:1140:GLY:HA2	1.76	0.51
1:B:215:ASP:OD1	1:B:215:ASP:N	2.42	0.50
1:A:131:VAL:HG23	1:A:133:THR:H	1.76	0.50
1:B:698:SER:O	1:B:702:ASN:ND2	2.45	0.50
1:B:1004:ILE:O	1:B:1008:PHE:HB2	2.11	0.50
1:C:987:ILE:HG22	1:C:992:VAL:HG21	1.93	0.50
1:A:214:ALA:HB2	1:A:220:THR:HA	1.93	0.50
1:A:1163:CYS:HB3	1:A:1214:LYS:HA	1.94	0.50
1:A:356:LEU:HD13	1:A:359:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ASN:N	1:B:531:ASN:OD1	2.44	0.50
1:B:789:GLN:NE2	1:B:1155:THR:OG1	2.43	0.50
1:C:1158:VAL:HB	1:C:1176:TYR:HB3	1.94	0.50
1:B:199:TYR:HB2	1:B:214:ALA:HB3	1.92	0.50
1:C:904:GLU:O	1:C:908:PHE:HB2	2.11	0.50
1:C:636:VAL:O	1:C:666:THR:OG1	2.30	0.50
1:C:396:ARG:NH1	1:C:578:ASP:OD2	2.45	0.50
1:C:955:ILE:HB	1:C:1136:ASN:HD21	1.77	0.50
1:C:904:GLU:OE1	1:C:1135:GLN:NE2	2.43	0.50
1:C:597:ILE:HD11	1:A:1064:ARG:HG2	1.93	0.49
1:C:1162:LEU:HD22	1:C:1218:ILE:HD12	1.94	0.49
1:B:850:LEU:HD13	1:B:1096:ILE:HD11	1.94	0.49
1:A:356:LEU:H	1:A:605:ASN:HD22	1.60	0.49
1:A:880:ASP:OD1	1:A:880:ASP:N	2.43	0.49
1:B:580:CYS:HB2	1:B:587:ASN:H	1.77	0.49
1:B:66:TYR:HB3	1:B:261:LEU:HD13	1.93	0.49
1:B:140:GLN:NE2	1:B:172:GLU:OE2	2.45	0.49
1:B:187:LYS:HD3	1:A:324:LEU:HD11	1.95	0.49
1:A:215:ASP:N	1:A:215:ASP:OD1	2.44	0.49
1:A:375:LYS:HA	1:A:378:ILE:HD12	1.95	0.49
1:C:108:ASN:HB3	1:C:196:ASP:HA	1.94	0.49
1:C:366:ASP:HB2	1:C:426:TYR:HB3	1.94	0.49
1:B:479:PRO:O	1:B:483:ASN:ND2	2.40	0.49
1:C:405:SER:O	1:C:415:LYS:NZ	2.46	0.49
1:B:688:PRO:O	1:B:722:ASN:ND2	2.40	0.49
1:C:558:THR:OG1	1:C:561:ASN:O	2.31	0.49
1:B:786:PHE:HD2	1:B:1158:VAL:HG23	1.77	0.49
1:A:481:VAL:HB	1:A:506:LEU:HD21	1.95	0.49
1:A:38:ASP:HB3	1:A:74:PHE:HB2	1.95	0.48
1:A:901:SER:H	1:A:904:GLU:HG3	1.78	0.48
1:B:568:SER:HB2	1:B:571:ALA:HB2	1.94	0.48
1:C:30:LYS:HA	1:C:88:LEU:HD22	1.96	0.48
1:C:90:TYR:OH	1:C:159:PRO:O	2.32	0.48
1:A:319:ARG:NE	1:A:660:ASP:OD1	2.46	0.48
1:C:1019:PHE:HA	1:C:1023:ASN:HD22	1.79	0.48
1:A:346:ARG:NH2	1:A:389:ASP:OD2	2.47	0.48
1:B:992:VAL:HG13	1:B:1191:TYR:HB2	1.95	0.48
1:C:444:TRP:NE1	1:C:547:PRO:O	2.46	0.48
1:A:142:HIS:NE2	1:A:147:GLU:OE1	2.43	0.48
1:A:422:SER:OG	1:A:424:GLN:NE2	2.47	0.48
1:A:654:ASN:OD1	1:A:654:ASN:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASN:HD22	1:B:31:THR:HB	1.80	0.47
1:B:1019:PHE:HB3	1:B:1026:LEU:HD11	1.94	0.47
1:C:385:SER:HB3	1:C:595:ASN:HB2	1.97	0.47
1:B:329:ILE:HA	1:B:332:TRP:HB3	1.96	0.47
1:C:18:PHE:HD2	2:I:1:NAG:H62	1.79	0.47
1:A:527:THR:OG1	1:A:528:TYR:N	2.47	0.47
1:C:794:PHE:HE1	1:C:1191:TYR:HB2	1.80	0.47
1:B:614:VAL:HG12	1:B:616:THR:HG22	1.97	0.47
1:A:369:SER:O	1:A:424:GLN:N	2.47	0.47
1:B:431:LEU:HD23	1:B:434:VAL:HG21	1.96	0.47
1:B:773:SER:HB2	1:C:866:THR:HG22	1.96	0.47
1:C:393:ILE:HD12	1:C:587:ASN:HB3	1.95	0.47
1:A:1107:ILE:O	1:A:1111:ASN:ND2	2.48	0.47
1:B:62:LEU:HD11	1:B:265:GLN:HE21	1.79	0.47
1:B:502:ARG:NH1	1:B:554:GLU:OE1	2.46	0.47
1:A:367:SER:HB3	1:A:426:TYR:HB2	1.97	0.47
1:C:161:THR:OG1	1:C:239:PRO:O	2.29	0.46
1:C:978:PRO:HG2	1:C:981:LEU:HB2	1.97	0.46
1:C:1061:ILE:HG23	1:C:1065:LEU:HD12	1.96	0.46
1:A:26:ASN:HB2	1:A:84:TYR:HB3	1.97	0.46
1:C:689:ALA:HA	1:C:722:ASN:HB3	1.97	0.46
1:C:919:VAL:O	1:C:923:ASN:ND2	2.48	0.46
1:A:69:LYS:NZ	1:A:70:SER:O	2.45	0.46
1:A:407:GLY:O	1:A:411:SER:OG	2.33	0.46
1:C:907:LEU:HD11	1:C:1142:LEU:HD22	1.98	0.46
1:A:728:SER:HG	4:A:2012:NAG:HO6	1.64	0.46
1:B:1208:CYS:HB2	1:B:1212:PHE:HD2	1.81	0.46
1:A:861:LEU:HB3	1:A:962:ALA:HB2	1.97	0.46
1:A:863:GLN:O	1:A:1115:LYS:NZ	2.48	0.46
1:B:772:VAL:HG12	1:C:865:VAL:HG13	1.98	0.46
1:B:952:GLU:HA	1:B:955:ILE:HB	1.97	0.46
1:C:118:TYR:HA	1:C:143:ASN:HD21	1.81	0.46
1:A:1047:LEU:HA	1:A:1081:ARG:HE	1.80	0.46
1:C:510:LEU:O	1:A:583:ASN:ND2	2.49	0.45
1:C:873:THR:HG1	1:C:891:LEU:H	1.64	0.45
1:A:1163:CYS:HB2	1:A:1212:PHE:HB3	1.98	0.45
1:B:38:ASP:H	1:B:73:ASN:HD21	1.63	0.45
1:A:794:PHE:HA	1:A:1150:PRO:HA	1.99	0.45
1:B:743:CYS:SG	1:B:744:ILE:N	2.89	0.45
1:B:870:ASN:OD1	1:B:870:ASN:N	2.49	0.45
1:C:956:SER:O	1:C:960:THR:OG1	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ASN:HA	1:C:429:LEU:HD11	1.98	0.45
1:A:172:GLU:OE2	1:A:174:TRP:NE1	2.48	0.45
1:C:800:GLU:HB2	1:C:1142:LEU:HD11	1.98	0.45
1:A:168:SER:OG	1:A:169:ILE:N	2.49	0.45
1:C:1169:GLY:N	1:C:1207:SER:O	2.50	0.45
1:A:937:VAL:O	1:A:941:ASN:ND2	2.40	0.45
1:B:794:PHE:HE2	1:B:1004:ILE:HD11	1.82	0.45
1:A:59:THR:OG1	1:A:60:THR:O	2.35	0.45
1:C:277:THR:OG1	1:C:278:ASN:OD1	2.33	0.45
1:C:438:ASN:ND2	1:C:459:ASP:O	2.46	0.44
1:A:358:THR:HA	1:A:361:ARG:HG2	1.99	0.44
1:A:969:PRO:HA	1:A:971:TRP:CD2	2.52	0.44
1:B:809:LYS:NZ	1:B:851:ASP:OD1	2.44	0.44
1:A:946:LEU:HD22	1:A:946:LEU:HA	1.87	0.44
1:B:95:LEU:HA	1:B:236:TYR:HB2	1.99	0.44
1:B:393:ILE:HD12	1:B:587:ASN:HB3	1.99	0.44
1:A:129:VAL:HB	1:A:131:VAL:HG22	1.99	0.44
1:C:91:LYS:HB3	1:C:93:PRO:HG2	1.99	0.44
1:B:802:PHE:HD2	1:B:1028:LYS:HB3	1.82	0.44
1:C:464:ASP:OD1	1:C:464:ASP:N	2.49	0.44
1:C:646:ASN:OD1	1:C:646:ASN:N	2.51	0.44
1:A:62:LEU:HD22	1:A:295:GLN:HE21	1.83	0.44
1:A:245:ILE:HG13	1:A:252:GLU:HB2	2.00	0.44
1:A:338:VAL:HB	1:A:436:ILE:HA	2.00	0.44
1:B:91:LYS:HD2	1:B:91:LYS:HA	1.70	0.44
1:C:415:LYS:HB3	1:C:542:ILE:HG12	1.98	0.44
1:C:431:LEU:HD11	1:C:581:ILE:HG21	1.99	0.44
1:A:556:CYS:HA	1:A:567:CYS:HA	2.00	0.44
1:B:671:PRO:HG2	1:C:940:PHE:HD2	1.83	0.44
1:B:1159:SER:HB3	1:B:1177:PHE:HB2	2.00	0.44
1:B:98:PHE:HB3	1:B:233:SER:HA	1.99	0.43
1:C:319:ARG:HA	1:C:319:ARG:HD2	1.88	0.43
1:A:608:LEU:HD13	1:A:608:LEU:HA	1.89	0.43
1:A:1151:THR:OG1	1:A:1152:SER:N	2.51	0.43
1:B:400:ASP:O	1:B:410:GLN:NE2	2.51	0.43
1:B:959:THR:O	1:B:963:THR:OG1	2.28	0.43
1:C:952:GLU:O	1:C:956:SER:OG	2.28	0.43
1:C:986:ARG:HD2	1:C:1117:GLN:HG2	1.99	0.43
1:C:312:LYS:HD3	1:C:312:LYS:HA	1.76	0.43
1:C:983:VAL:O	1:C:987:ILE:HG13	2.18	0.43
1:A:417:ASP:HB2	1:A:542:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:SER:OG	1:B:73:ASN:ND2	2.51	0.43
1:B:161:THR:HA	1:B:172:GLU:HG3	2.01	0.43
1:B:951:SER:OG	1:B:954:GLN:OE1	2.37	0.43
1:C:850:LEU:HD13	1:C:1096:ILE:HD11	2.00	0.43
1:C:885:LYS:HE3	1:C:885:LYS:HB2	1.87	0.43
1:A:846:VAL:HG13	1:A:1096:ILE:HG13	2.00	0.43
1:B:777:ASP:HB3	1:B:787:GLU:HB3	2.00	0.43
1:B:901:SER:O	1:B:905:ASP:N	2.51	0.43
1:C:491:LEU:HD22	1:C:559:GLN:HB2	2.00	0.43
1:A:319:ARG:HB2	1:A:624:LEU:HD23	2.01	0.43
1:A:722:ASN:OD1	1:A:760:SER:OG	2.36	0.43
1:B:139:VAL:HG13	1:B:148:ILE:HG12	2.01	0.43
1:A:505:ASP:HB2	1:A:517:ARG:HG3	2.01	0.43
1:B:74:PHE:CG	1:B:257:TRP:HB3	2.54	0.43
1:C:16:GLY:HA3	1:C:155:MET:HB2	2.01	0.43
1:A:203:TYR:HB3	1:A:261:LEU:HD12	2.01	0.43
1:B:767:PHE:O	1:C:954:GLN:NE2	2.50	0.43
1:B:983:VAL:HG22	1:B:1131:LEU:HD21	2.01	0.43
1:C:785:LEU:HD12	1:C:1157:LEU:HD12	2.01	0.43
1:C:849:LEU:O	1:C:853:THR:OG1	2.35	0.43
1:A:1165:SER:OG	1:A:1218:ILE:O	2.34	0.43
1:B:392:ALA:HB3	1:B:460:VAL:HG11	2.01	0.43
1:A:1066:ASP:O	1:A:1070:ALA:N	2.51	0.43
1:B:1196:PRO:O	1:B:1201:ASN:ND2	2.52	0.42
1:C:163:CYS:HB3	1:C:240:LEU:HD21	2.00	0.42
1:B:378:ILE:HG23	1:B:383:PHE:HZ	1.85	0.42
1:B:711:PHE:HE1	1:B:758:ILE:HB	1.84	0.42
1:B:917:GLY:HA2	1:B:920:GLU:HG2	2.00	0.42
1:A:518:CYS:H	1:A:521:LEU:HD11	1.84	0.42
1:B:320:ARG:HH22	1:B:626:GLY:HA2	1.83	0.42
1:B:593:ILE:O	1:B:595:ASN:ND2	2.52	0.42
1:C:981:LEU:HA	1:C:984:GLN:HB2	2.01	0.42
1:A:648:LEU:HD12	1:A:648:LEU:HA	1.94	0.42
1:B:472:ASP:HB2	1:B:500:LYS:HG3	2.01	0.42
1:C:687:SER:O	1:C:762:TYR:OH	2.36	0.42
1:C:1047:LEU:O	1:C:1056:SER:OG	2.26	0.42
1:A:312:LYS:HD3	1:A:312:LYS:HA	1.85	0.42
1:C:648:LEU:HA	1:A:55:VAL:HB	2.00	0.42
1:B:109:THR:OG1	1:B:120:GLU:O	2.38	0.42
1:A:369:SER:HB3	1:A:424:GLN:HB2	2.00	0.42
1:A:445:ASN:OD1	1:A:549:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:801:GLU:OE2	1:B:1145:HIS:NE2	2.47	0.42
1:B:816:ALA:HA	1:B:820:SER:HA	2.01	0.42
1:C:861:LEU:HA	1:C:1115:LYS:HE3	2.02	0.42
1:A:329:ILE:HG21	1:A:388:VAL:HG21	2.01	0.42
1:B:869:SER:OG	1:A:775:VAL:O	2.28	0.42
1:C:1145:HIS:O	1:C:1147:SER:OG	2.37	0.42
1:A:805:THR:HG22	1:A:1103:ALA:HA	2.02	0.42
1:B:931:ILE:HD11	1:A:656:ILE:HD12	2.01	0.42
1:B:128:SER:HB2	1:B:232:LEU:HA	2.02	0.41
1:B:1178:ILE:H	1:B:1178:ILE:HG13	1.74	0.41
1:A:466:CYS:HB3	1:A:547:PRO:HD2	2.02	0.41
1:A:865:VAL:HG21	1:A:965:ALA:HB1	2.01	0.41
1:B:964:VAL:HG23	1:B:967:MET:HE1	2.02	0.41
1:B:982:ASN:OD1	1:B:1117:GLN:NE2	2.54	0.41
1:A:552:ASN:H	1:A:571:ALA:HB1	1.85	0.41
1:B:98:PHE:HE2	1:B:101:GLY:HA2	1.84	0.41
1:B:314:VAL:H	1:B:620:VAL:HA	1.85	0.41
1:C:780:GLU:H	1:C:780:GLU:HG2	1.70	0.41
1:A:378:ILE:HG12	1:A:383:PHE:HZ	1.85	0.41
1:A:795:THR:OG1	1:A:796:ILE:N	2.54	0.41
1:A:1170:ILE:HG22	1:A:1204:PHE:HA	2.02	0.41
1:B:98:PHE:HB2	1:B:235:TYR:HD2	1.85	0.41
1:B:965:ALA:HB1	1:B:972:SER:HB2	2.02	0.41
1:B:990:LEU:O	1:B:1190:SER:OG	2.33	0.41
1:C:112:TYR:HD1	1:C:112:TYR:HA	1.73	0.41
1:C:647:LEU:O	1:A:55:VAL:N	2.49	0.41
1:C:1121:ILE:H	1:C:1121:ILE:HG13	1.65	0.41
1:A:865:VAL:HG23	1:A:972:SER:HB2	2.01	0.41
1:B:212:TYR:HB3	1:B:220:THR:HB	2.02	0.41
1:B:1178:ILE:HG12	1:B:1187:THR:HB	2.02	0.41
1:C:1148:TYR:OH	1:C:1190:SER:O	2.38	0.41
1:A:515:TRP:HE1	1:A:517:ARG:HD2	1.85	0.41
1:A:537:LYS:HE3	1:A:537:LYS:HB2	1.90	0.41
1:A:1201:ASN:OD1	1:A:1201:ASN:N	2.52	0.41
1:C:164:LYS:HE2	1:C:164:LYS:HB3	1.83	0.41
1:C:355:ASN:ND2	1:C:605:ASN:OD1	2.50	0.41
1:C:360:LEU:HD23	1:C:360:LEU:HA	1.95	0.41
1:C:987:ILE:HD12	1:C:997:LEU:HD21	2.03	0.41
1:A:961:ALA:O	1:A:965:ALA:HB2	2.21	0.41
1:A:1149:LYS:HA	1:A:1150:PRO:HD3	1.95	0.41
1:B:572:PHE:O	1:B:575:TRP:NE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:NH2	1:C:380:GLY:O	2.54	0.41
1:C:1015:ILE:HD13	1:C:1015:ILE:HA	1.86	0.41
1:C:1191:TYR:CD1	1:C:1193:TYR:HB2	2.55	0.41
1:C:832:TYR:OH	1:C:1079:ASN:ND2	2.52	0.41
1:A:115:ASN:OD1	1:A:115:ASN:N	2.53	0.41
1:A:1163:CYS:O	1:A:1215:ALA:N	2.46	0.41
1:B:332:TRP:HA	1:B:335:ASN:HB2	2.02	0.41
1:C:223:LEU:HD12	1:C:223:LEU:HA	1.90	0.41
1:C:748:LEU:H	1:C:748:LEU:HG	1.45	0.41
1:C:961:ALA:HA	1:C:964:VAL:HG12	2.02	0.41
1:A:790:ILE:HB	1:A:1192:TYR:HB2	2.03	0.41
1:A:839:ILE:HG23	1:A:1089:VAL:HG21	2.02	0.41
1:B:219:PRO:HG2	1:B:276:ILE:HD12	2.02	0.40
1:C:405:SER:OG	1:C:406:SER:N	2.54	0.40
1:C:238:MET:HE3	1:C:238:MET:HB2	1.92	0.40
1:C:1018:GLY:O	1:C:1023:ASN:ND2	2.55	0.40
1:C:1220:LEU:HD13	1:C:1220:LEU:HA	1.96	0.40
1:B:30:LYS:H	1:B:30:LYS:HG2	1.73	0.40
1:C:616:THR:HG21	1:C:635:GLU:HB2	2.03	0.40
1:A:642:ASN:OD1	1:A:643:ASN:ND2	2.54	0.40
1:B:789:GLN:NE2	1:B:1155:THR:HG1	2.19	0.40
1:A:130:PHE:HA	1:A:136:THR:HG21	2.03	0.40
1:A:1061:ILE:HG23	1:A:1065:LEU:HD12	2.03	0.40
1:C:898:SER:O	1:C:898:SER:OG	2.39	0.40
1:A:465:HIS:HE1	1:A:537:LYS:HD3	1.86	0.40
1:A:1067:PRO:O	1:A:1071:GLN:NE2	2.45	0.40
1:A:1130:ILE:HG22	1:A:1131:LEU:HG	2.04	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%)	1097 (91%)	109 (9%)	0	100	100
1	B	1206/1290 (94%)	1125 (93%)	81 (7%)	0	100	100
1	C	1206/1290 (94%)	1105 (92%)	101 (8%)	0	100	100
All	All	3618/3870 (94%)	3327 (92%)	291 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1082/1159 (93%)	933 (86%)	149 (14%)	3	16
1	B	1082/1159 (93%)	910 (84%)	172 (16%)	2	11
1	C	1082/1159 (93%)	908 (84%)	174 (16%)	2	11
All	All	3246/3477 (93%)	2751 (85%)	495 (15%)	5	12

All (495) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	VAL
1	B	21	THR
1	B	25	ILE
1	B	29	ASN
1	B	34	ARG
1	B	37	GLU
1	B	38	ASP
1	B	40	VAL
1	B	50	TYR
1	B	54	ARG
1	B	55	VAL
1	B	73	ASN
1	B	85	LEU
1	B	88	LEU
1	B	91	LYS

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Mol	Chain	Res	Type
1	B	99	ASN
1	B	100	ASN
1	B	102	ILE
1	B	117	LEU
1	B	123	THR
1	B	124	ILE
1	B	125	VAL
1	B	129	VAL
1	B	131	VAL
1	B	136	THR
1	B	145	ILE
1	B	146	LEU
1	B	149	THR
1	B	153	TYR
1	B	157	GLU
1	B	162	VAL
1	B	166	LYS
1	B	177	ASP
1	B	203	TYR
1	B	204	GLN
1	B	216	VAL
1	B	231	ILE
1	B	243	LYS
1	B	247	SER
1	B	249	THR
1	B	254	LEU
1	B	258	VAL
1	B	261	LEU
1	B	264	ARG
1	B	266	TYR
1	B	275	VAL
1	B	276	ILE
1	B	277	THR
1	B	280	VAL
1	B	282	CYS
1	B	283	SER
1	B	285	SER
1	B	287	LEU
1	B	289	GLU
1	B	309	PHE
1	B	317	VAL
1	B	320	ARG

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Mol	Chain	Res	Type
1	B	331	ASN
1	B	346	ARG
1	B	358	THR
1	B	359	LEU
1	B	373	LEU
1	B	399	ASP
1	B	403	LEU
1	B	428	SER
1	B	429	LEU
1	B	450	PHE
1	B	455	VAL
1	B	472	ASP
1	B	480	SER
1	B	482	VAL
1	B	485	CYS
1	B	486	VAL
1	B	503	HIS
1	B	506	LEU
1	B	512	VAL
1	B	517	ARG
1	B	523	ASP
1	B	526	SER
1	B	531	ASN
1	B	540	VAL
1	B	544	GLU
1	B	558	THR
1	B	582	SER
1	B	601	THR
1	B	603	CYS
1	B	604	SER
1	B	616	THR
1	B	618	VAL
1	B	621	ASN
1	B	640	TYR
1	B	655	ILE
1	B	658	PHE
1	B	659	LYS
1	B	662	LEU
1	B	677	VAL
1	B	706	PHE
1	B	711	PHE
1	B	714	ASP

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Mol	Chain	Res	Type
1	B	731	VAL
1	B	735	ASP
1	B	737	ARG
1	B	740	SER
1	B	743	CYS
1	B	748	LEU
1	B	758	ILE
1	B	760	SER
1	B	772	VAL
1	B	787	GLU
1	B	788	ILE
1	B	801	GLU
1	B	828	LEU
1	B	835	PHE
1	B	848	ASP
1	B	849	LEU
1	B	850	LEU
1	B	852	ILE
1	B	865	VAL
1	B	866	THR
1	B	869	SER
1	B	870	ASN
1	B	871	LEU
1	B	875	LEU
1	B	879	VAL
1	B	880	ASP
1	B	887	LEU
1	B	888	LEU
1	B	890	CYS
1	B	903	LEU
1	B	931	ILE
1	B	932	ARG
1	B	950	LEU
1	B	951	SER
1	B	952	GLU
1	B	963	THR
1	B	967	MET
1	B	986	ARG
1	B	987	ILE
1	B	988	ASN
1	B	990	LEU
1	B	992	VAL

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Mol	Chain	Res	Type
1	B	993	THR
1	B	995	ASP
1	B	1001	GLN
1	B	1002	LYS
1	B	1010	LYS
1	B	1012	LEU
1	B	1015	ILE
1	B	1017	ASN
1	B	1022	THR
1	B	1030	GLN
1	B	1031	SER
1	B	1066	ASP
1	B	1075	ASP
1	B	1086	ASN
1	B	1089	VAL
1	B	1096	ILE
1	B	1098	LEU
1	B	1113	CYS
1	B	1115	LYS
1	B	1124	CYS
1	B	1129	HIS
1	B	1131	LEU
1	B	1157	LEU
1	B	1173	LYS
1	B	1178	ILE
1	B	1189	SER
1	B	1193	TYR
1	B	1195	GLU
1	B	1203	VAL
1	B	1207	SER
1	B	1217	PHE
1	C	14	VAL
1	C	20	CYS
1	C	21	THR
1	C	22	ASN
1	C	25	ILE
1	C	26	ASN
1	C	29	ASN
1	C	30	LYS
1	C	31	THR
1	C	34	ARG
1	C	37	GLU

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Mol	Chain	Res	Type
1	C	41	ASP
1	C	42	VAL
1	C	51	VAL
1	C	52	LEU
1	C	59	THR
1	C	69	LYS
1	C	74	PHE
1	C	76	ASP
1	C	77	LEU
1	C	112	TYR
1	C	114	ASN
1	C	123	THR
1	C	125	VAL
1	C	129	VAL
1	C	132	ASN
1	C	147	GLU
1	C	149	THR
1	C	153	TYR
1	C	154	THR
1	C	161	THR
1	C	182	LEU
1	C	187	LYS
1	C	189	PHE
1	C	205	GLU
1	C	206	ARG
1	C	226	LEU
1	C	228	LEU
1	C	233	SER
1	C	243	LYS
1	C	248	ASN
1	C	258	VAL
1	C	259	THR
1	C	262	SER
1	C	272	GLU
1	C	275	VAL
1	C	278	ASN
1	C	280	VAL
1	C	282	CYS
1	C	294	THR
1	C	303	VAL
1	C	309	PHE
1	C	311	VAL

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Mol	Chain	Res	Type
1	C	328	ASP
1	C	330	ASP
1	C	373	LEU
1	C	374	ASP
1	C	375	LYS
1	C	378	ILE
1	C	403	LEU
1	C	426	TYR
1	C	434	VAL
1	C	460	VAL
1	C	464	ASP
1	C	472	ASP
1	C	481	VAL
1	C	491	LEU
1	C	505	ASP
1	C	511	TYR
1	C	512	VAL
1	C	516	CYS
1	C	520	CYS
1	C	527	THR
1	C	535	GLN
1	C	540	VAL
1	C	549	LEU
1	C	558	THR
1	C	560	LEU
1	C	573	LEU
1	C	581	ILE
1	C	597	ILE
1	C	601	THR
1	C	606	ASP
1	C	618	VAL
1	C	621	ASN
1	C	652	ASN
1	C	656	ILE
1	C	659	LYS
1	C	661	PHE
1	C	706	PHE
1	C	728	SER
1	C	734	CYS
1	C	748	LEU
1	C	756	ARG
1	C	775	VAL

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Mol	Chain	Res	Type
1	C	780	GLU
1	C	781	THR
1	C	792	THR
1	C	794	PHE
1	C	795	THR
1	C	796	ILE
1	C	800	GLU
1	C	805	THR
1	C	811	THR
1	C	820	SER
1	C	821	ASN
1	C	828	LEU
1	C	849	LEU
1	C	850	LEU
1	C	853	THR
1	C	865	VAL
1	C	867	LEU
1	C	871	LEU
1	C	873	THR
1	C	875	LEU
1	C	878	ASP
1	C	879	VAL
1	C	880	ASP
1	C	885	LYS
1	C	886	SER
1	C	890	CYS
1	C	894	GLN
1	C	899	SER
1	C	930	GLU
1	C	952	GLU
1	C	953	THR
1	C	964	VAL
1	C	967	MET
1	C	977	VAL
1	C	981	LEU
1	C	983	VAL
1	C	993	THR
1	C	996	VAL
1	C	997	LEU
1	C	1002	LYS
1	C	1012	LEU
1	C	1015	ILE

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Mol	Chain	Res	Type
1	C	1022	THR
1	C	1056	SER
1	C	1066	ASP
1	C	1069	GLU
1	C	1072	VAL
1	C	1077	LEU
1	C	1086	ASN
1	C	1089	VAL
1	C	1095	ASP
1	C	1096	ILE
1	C	1098	LEU
1	C	1113	CYS
1	C	1115	LYS
1	C	1121	ILE
1	C	1131	LEU
1	C	1133	LEU
1	C	1141	LEU
1	C	1147	SER
1	C	1151	THR
1	C	1154	LYS
1	C	1157	LEU
1	C	1159	SER
1	C	1162	LEU
1	C	1163	CYS
1	C	1178	ILE
1	C	1179	LYS
1	C	1187	THR
1	C	1195	GLU
1	C	1199	ASP
1	C	1202	VAL
1	C	1203	VAL
1	C	1206	ASN
1	C	1208	CYS
1	C	1209	SER
1	C	1212	PHE
1	C	1213	THR
1	C	1220	LEU
1	A	14	VAL
1	A	18	PHE
1	A	21	THR
1	A	28	TYR
1	A	34	ARG

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Mol	Chain	Res	Type
1	A	35	ILE
1	A	43	SER
1	A	48	THR
1	A	51	VAL
1	A	60	THR
1	A	64	THR
1	A	75	ARG
1	A	96	SER
1	A	97	ASP
1	A	109	THR
1	A	112	TYR
1	A	115	ASN
1	A	116	THR
1	A	124	ILE
1	A	125	VAL
1	A	129	VAL
1	A	134	SER
1	A	145	ILE
1	A	182	LEU
1	A	187	LYS
1	A	204	GLN
1	A	208	VAL
1	A	213	TYR
1	A	241	THR
1	A	243	LYS
1	A	245	ILE
1	A	248	ASN
1	A	253	THR
1	A	258	VAL
1	A	259	THR
1	A	263	ARG
1	A	268	LEU
1	A	277	THR
1	A	305	ASP
1	A	306	LEU
1	A	310	THR
1	A	311	VAL
1	A	312	LYS
1	A	314	VAL
1	A	317	VAL
1	A	318	TYR
1	A	358	THR

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Mol	Chain	Res	Type
1	A	360	LEU
1	A	366	ASP
1	A	418	ILE
1	A	429	LEU
1	A	432	VAL
1	A	482	VAL
1	A	503	HIS
1	A	515	TRP
1	A	525	ILE
1	A	528	TYR
1	A	540	VAL
1	A	542	ILE
1	A	560	LEU
1	A	573	LEU
1	A	588	ILE
1	A	597	ILE
1	A	601	THR
1	A	608	LEU
1	A	619	CYS
1	A	644	TRP
1	A	646	ASN
1	A	654	ASN
1	A	655	ILE
1	A	662	LEU
1	A	666	THR
1	A	676	ARG
1	A	677	VAL
1	A	685	SER
1	A	706	PHE
1	A	707	ILE
1	A	714	ASP
1	A	726	LEU
1	A	734	CYS
1	A	737	ARG
1	A	748	LEU
1	A	765	VAL
1	A	772	VAL
1	A	778	SER
1	A	779	VAL
1	A	781	THR
1	A	782	VAL
1	A	790	ILE

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Mol	Chain	Res	Type
1	A	792	THR
1	A	799	HIS
1	A	801	GLU
1	A	803	ILE
1	A	811	THR
1	A	835	PHE
1	A	848	ASP
1	A	849	LEU
1	A	850	LEU
1	A	862	MET
1	A	866	THR
1	A	871	LEU
1	A	875	LEU
1	A	879	VAL
1	A	880	ASP
1	A	888	LEU
1	A	904	GLU
1	A	907	LEU
1	A	930	GLU
1	A	932	ARG
1	A	934	LEU
1	A	946	LEU
1	A	953	THR
1	A	977	VAL
1	A	981	LEU
1	A	983	VAL
1	A	987	ILE
1	A	990	LEU
1	A	994	MET
1	A	996	VAL
1	A	1001	GLN
1	A	1002	LYS
1	A	1003	LEU
1	A	1004	ILE
1	A	1012	LEU
1	A	1013	LEU
1	A	1023	ASN
1	A	1026	LEU
1	A	1057	SER
1	A	1066	ASP
1	A	1069	GLU
1	A	1086	ASN

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Mol	Chain	Res	Type
1	A	1089	VAL
1	A	1096	ILE
1	A	1098	LEU
1	A	1104	SER
1	A	1114	VAL
1	A	1117	GLN
1	A	1131	LEU
1	A	1147	SER
1	A	1149	LYS
1	A	1156	VAL
1	A	1176	TYR
1	A	1178	ILE
1	A	1187	THR
1	A	1203	VAL
1	A	1205	MET
1	A	1210	VAL
1	A	1219	TYR
1	A	1221	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	26	ASN
1	B	73	ASN
1	B	99	ASN
1	B	140	GLN
1	B	152	GLN
1	B	265	GLN
1	B	343	ASN
1	B	371	ASN
1	B	402	GLN
1	B	503	HIS
1	B	598	ASN
1	B	621	ASN
1	B	694	ASN
1	B	789	GLN
1	B	821	ASN
1	B	856	GLN
1	B	876	HIS
1	B	982	ASN
1	B	984	GLN
1	B	1000	ASN

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Mol	Chain	Res	Type
1	B	1017	ASN
1	B	1045	GLN
1	B	1091	GLN
1	B	1117	GLN
1	B	1122	ASN
1	B	1174	GLN
1	B	1201	ASN
1	C	22	ASN
1	C	115	ASN
1	C	140	GLN
1	C	142	HIS
1	C	152	GLN
1	C	204	GLN
1	C	248	ASN
1	C	269	ASN
1	C	351	ASN
1	C	562	HIS
1	C	643	ASN
1	C	694	ASN
1	C	722	ASN
1	C	870	ASN
1	C	874	ASN
1	C	876	HIS
1	C	923	ASN
1	C	1000	ASN
1	C	1045	GLN
1	C	1073	GLN
1	C	1091	GLN
1	C	1136	ASN
1	A	201	HIS
1	A	204	GLN
1	A	265	GLN
1	A	273	HIS
1	A	278	ASN
1	A	295	GLN
1	A	465	HIS
1	A	561	ASN
1	A	584	ASN
1	A	595	ASN
1	A	605	ASN
1	A	643	ASN
1	A	854	GLN

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Mol	Chain	Res	Type
1	A	859	ASN
1	A	1000	ASN
1	A	1023	ASN
1	A	1049	ASN
1	A	1059	GLN
1	A	1079	ASN
1	A	1091	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.39	0	17,19,21	0.52	0
2	NAG	D	2	2	14,14,15	0.29	0	17,19,21	0.50	0
2	MAN	D	3	2	11,11,12	1.46	2 (18%)	15,15,17	1.48	2 (13%)
2	MAN	D	4	2	11,11,12	0.91	1 (9%)	15,15,17	1.22	2 (13%)
2	MAN	D	5	2	11,11,12	0.92	0	15,15,17	0.91	2 (13%)
2	MAN	D	6	2	11,11,12	0.98	1 (9%)	15,15,17	1.42	2 (13%)
3	NAG	E	1	1,3	14,14,15	0.55	0	17,19,21	0.64	0
3	NAG	E	2	3	14,14,15	0.50	0	17,19,21	0.47	0
3	NAG	F	1	1,3	14,14,15	0.31	0	17,19,21	0.51	0
3	NAG	F	2	3	14,14,15	0.37	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	1	1,3	14,14,15	0.79	1 (7%)	17,19,21	1.09	1 (5%)
3	NAG	G	2	3	14,14,15	0.44	0	17,19,21	0.65	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.29	0	17,19,21	0.57	0
3	NAG	H	2	3	14,14,15	0.33	0	17,19,21	0.50	0
2	NAG	I	1	2,1	14,14,15	0.40	0	17,19,21	0.73	1 (5%)
2	NAG	I	2	2	14,14,15	0.29	0	17,19,21	0.56	0
2	MAN	I	3	2	11,11,12	1.36	1 (9%)	15,15,17	1.72	3 (20%)
2	MAN	I	4	2	11,11,12	0.94	1 (9%)	15,15,17	1.38	2 (13%)
2	MAN	I	5	2	11,11,12	1.16	1 (9%)	15,15,17	1.43	3 (20%)
2	MAN	I	6	2	11,11,12	1.42	2 (18%)	15,15,17	2.22	4 (26%)
3	NAG	J	1	1,3	14,14,15	0.38	0	17,19,21	0.53	0
3	NAG	J	2	3	14,14,15	0.40	0	17,19,21	0.45	0
3	NAG	K	1	1,3	14,14,15	0.23	0	17,19,21	0.52	0
3	NAG	K	2	3	14,14,15	0.31	0	17,19,21	0.54	0
3	NAG	L	1	1,3	14,14,15	0.40	0	17,19,21	0.59	0
3	NAG	L	2	3	14,14,15	0.40	0	17,19,21	0.47	0
3	NAG	M	1	1,3	14,14,15	0.42	0	17,19,21	0.44	0
3	NAG	M	2	3	14,14,15	0.42	0	17,19,21	0.59	1 (5%)
2	NAG	N	1	2,1	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	N	2	2	14,14,15	0.37	0	17,19,21	0.52	0
2	MAN	N	3	2	11,11,12	1.80	4 (36%)	15,15,17	1.58	3 (20%)
2	MAN	N	4	2	11,11,12	1.04	0	15,15,17	0.98	1 (6%)
2	MAN	N	5	2	11,11,12	0.94	1 (9%)	15,15,17	1.24	2 (13%)
2	MAN	N	6	2	11,11,12	0.73	0	15,15,17	1.25	2 (13%)
3	NAG	O	1	1,3	14,14,15	0.39	0	17,19,21	0.62	0
3	NAG	O	2	3	14,14,15	0.32	0	17,19,21	0.41	0
3	NAG	P	1	1,3	14,14,15	0.23	0	17,19,21	0.51	0
3	NAG	P	2	3	14,14,15	0.39	0	17,19,21	0.58	0
3	NAG	Q	1	1,3	14,14,15	0.62	0	17,19,21	0.97	1 (5%)
3	NAG	Q	2	3	14,14,15	0.46	0	17,19,21	0.54	0
3	NAG	R	1	1,3	14,14,15	0.21	0	17,19,21	0.61	0
3	NAG	R	2	3	14,14,15	0.37	0	17,19,21	0.48	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	-	1/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	MAN	O5-C5	3.52	1.50	1.43
2	N	3	MAN	O5-C5	3.47	1.50	1.43
2	I	6	MAN	C1-C2	3.16	1.59	1.52
2	I	5	MAN	C1-C2	3.11	1.59	1.52
2	N	3	MAN	C1-C2	2.89	1.59	1.52
2	I	3	MAN	O5-C5	2.79	1.48	1.43
2	I	6	MAN	C2-C3	2.55	1.56	1.52
2	D	6	MAN	C1-C2	2.52	1.58	1.52
3	G	1	NAG	O5-C1	2.50	1.47	1.43
2	D	3	MAN	C1-C2	2.27	1.57	1.52
2	N	5	MAN	C1-C2	2.26	1.57	1.52
2	N	3	MAN	C2-C3	2.25	1.55	1.52
2	N	3	MAN	C4-C3	2.24	1.58	1.52
2	D	4	MAN	C1-C2	2.18	1.57	1.52
2	I	4	MAN	O5-C5	2.12	1.47	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	6	MAN	C1-O5-C5	6.46	120.84	112.19
2	I	3	MAN	C1-O5-C5	5.38	119.39	112.19
2	N	3	MAN	C1-O5-C5	4.62	118.38	112.19
2	D	3	MAN	C1-O5-C5	4.30	117.95	112.19
2	D	6	MAN	C1-O5-C5	4.29	117.93	112.19
2	N	6	MAN	C1-O5-C5	3.87	117.37	112.19
2	I	6	MAN	C1-C2-C3	3.73	115.08	109.64
2	I	4	MAN	C1-O5-C5	3.64	117.07	112.19
2	I	5	MAN	C1-O5-C5	3.61	117.02	112.19
2	N	5	MAN	C1-O5-C5	3.46	116.83	112.19
3	G	1	NAG	C1-O5-C5	3.36	116.69	112.19
2	D	4	MAN	C1-O5-C5	3.23	116.51	112.19
3	Q	1	NAG	C1-O5-C5	3.04	116.26	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	6	MAN	O5-C1-C2	2.50	116.75	110.79
2	N	3	MAN	O2-C2-C3	-2.42	105.14	110.15
2	D	3	MAN	O2-C2-C3	-2.35	105.28	110.15
3	G	2	NAG	C1-O5-C5	2.32	115.30	112.19
2	I	5	MAN	C1-C2-C3	2.32	113.02	109.64
2	D	5	MAN	O2-C2-C3	-2.25	105.49	110.15
2	N	6	MAN	O2-C2-C3	-2.25	105.49	110.15
2	N	4	MAN	O2-C2-C3	-2.20	105.59	110.15
2	D	4	MAN	O2-C2-C3	-2.17	105.66	110.15
2	I	5	MAN	O2-C2-C3	-2.16	105.68	110.15
2	D	6	MAN	O2-C2-C3	-2.15	105.69	110.15
2	N	3	MAN	C1-C2-C3	2.14	112.77	109.64
2	I	1	NAG	C1-O5-C5	2.13	115.03	112.19
2	I	6	MAN	O2-C2-C3	-2.12	105.75	110.15
2	I	3	MAN	O2-C2-C3	-2.10	105.81	110.15
2	I	3	MAN	C2-C3-C4	2.06	114.48	110.86
2	N	5	MAN	O2-C2-C3	-2.06	105.89	110.15
2	I	4	MAN	O2-C2-C3	-2.05	105.91	110.15
3	M	2	NAG	C1-O5-C5	2.03	114.91	112.19
2	D	5	MAN	C1-O5-C5	2.02	114.90	112.19

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
2	N	3	MAN	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

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

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Mol	Chain	Res	Type	Atoms
3	O	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6

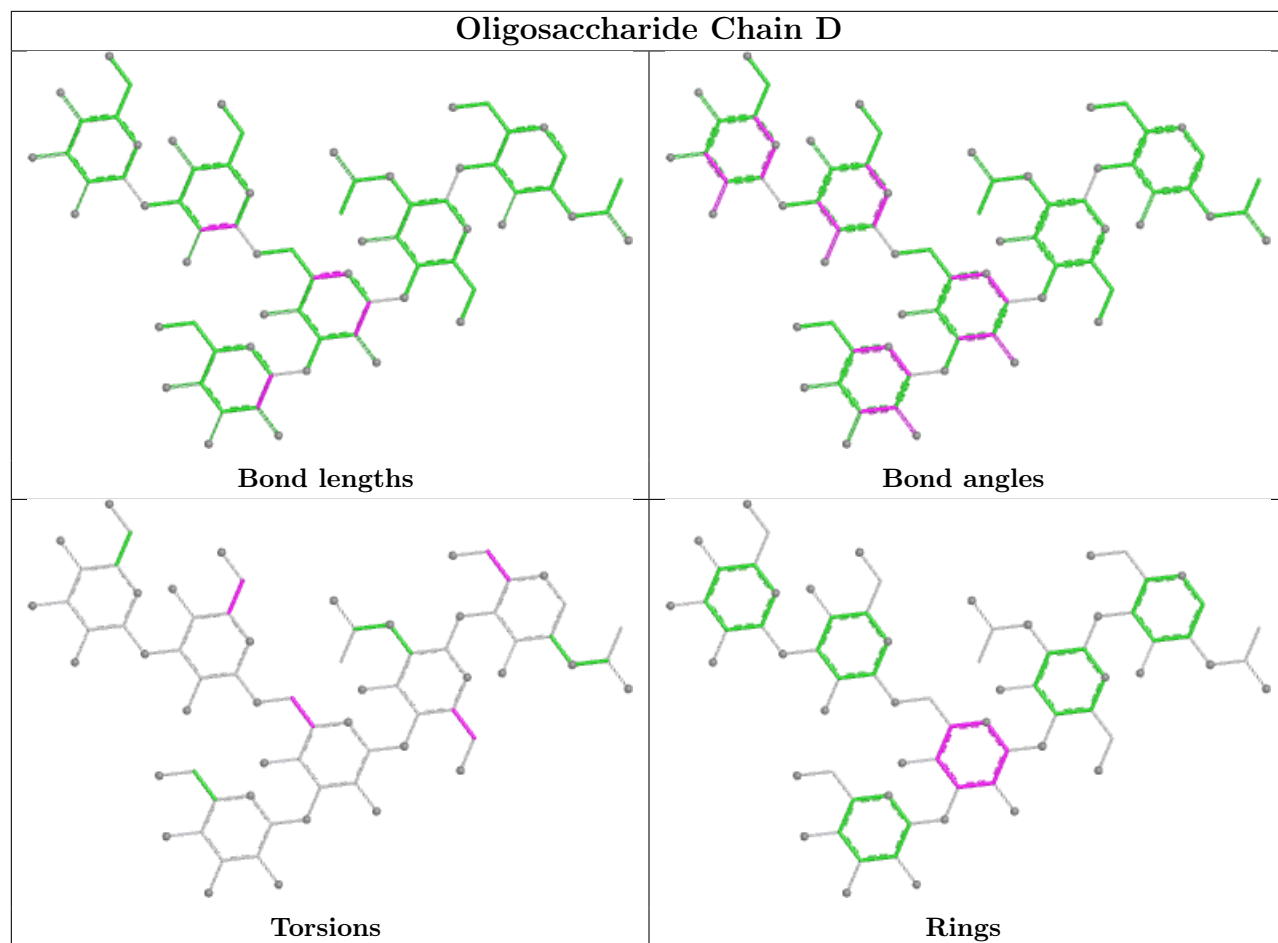
All (2) ring outliers are listed below:

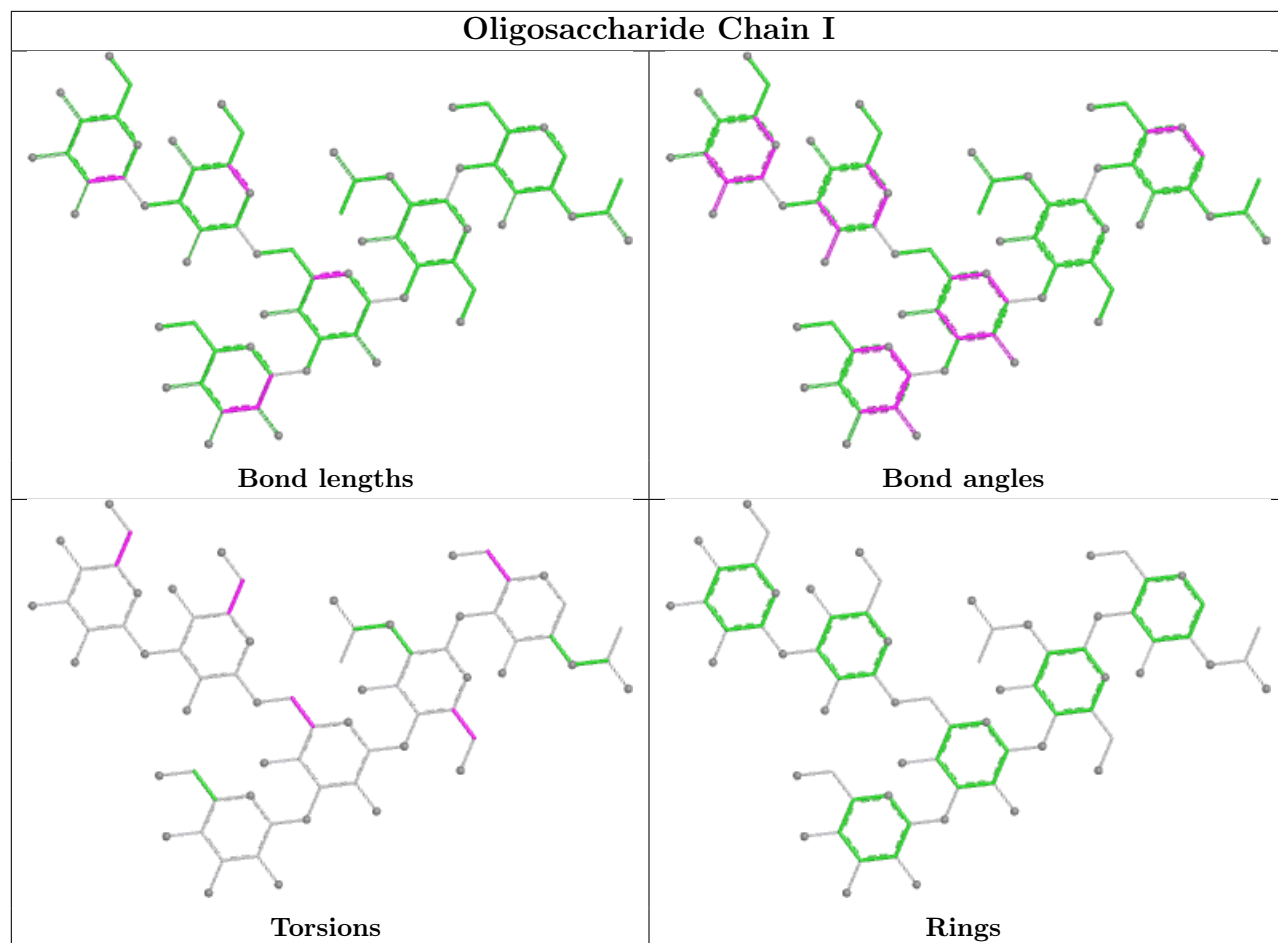
Mol	Chain	Res	Type	Atoms
2	N	3	MAN	C1-C2-C3-C4-C5-O5
2	D	3	MAN	C1-C2-C3-C4-C5-O5

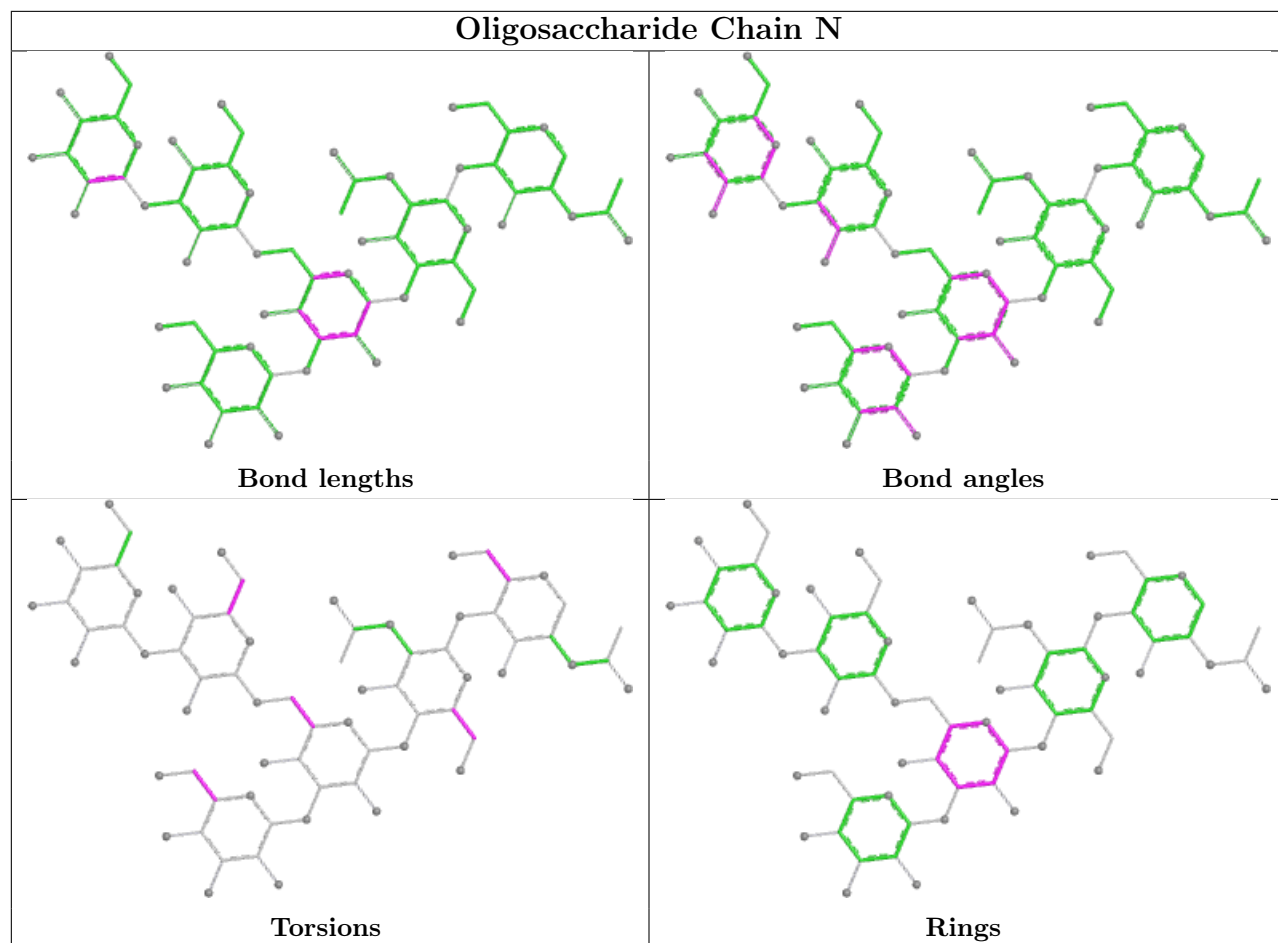
3 monomers are involved in 3 short contacts:

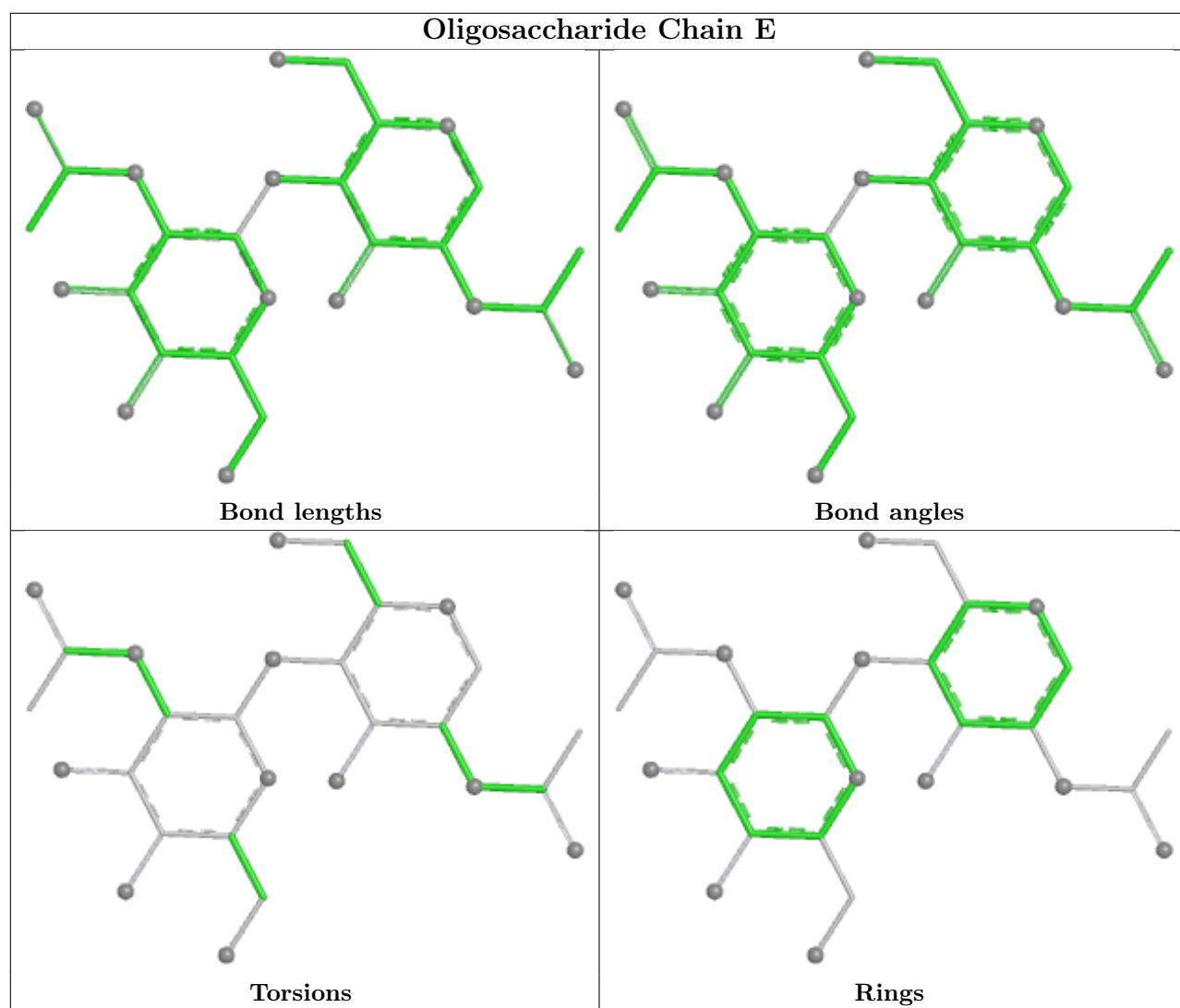
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
3	G	1	NAG	1	0
2	I	1	NAG	1	0

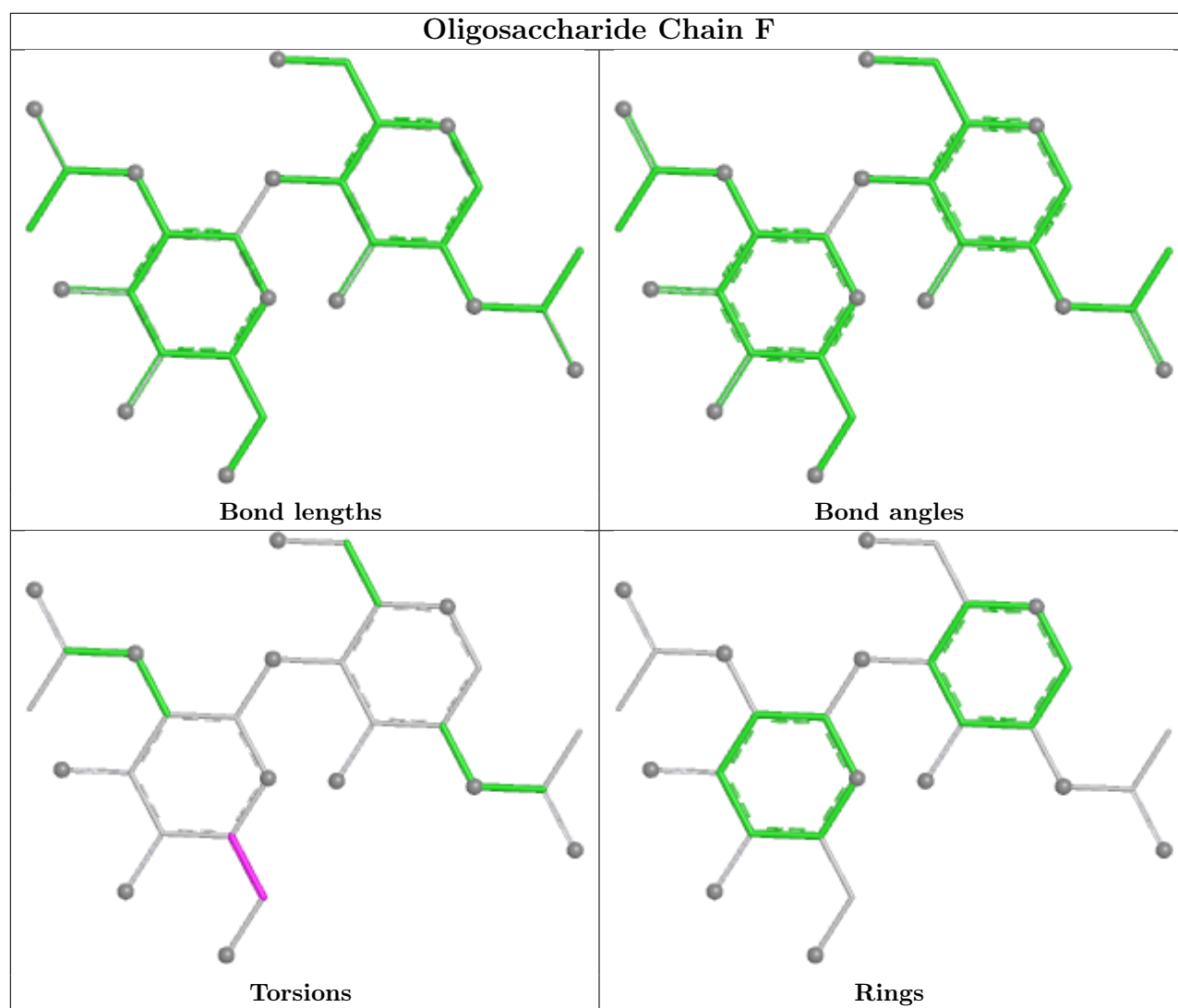
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

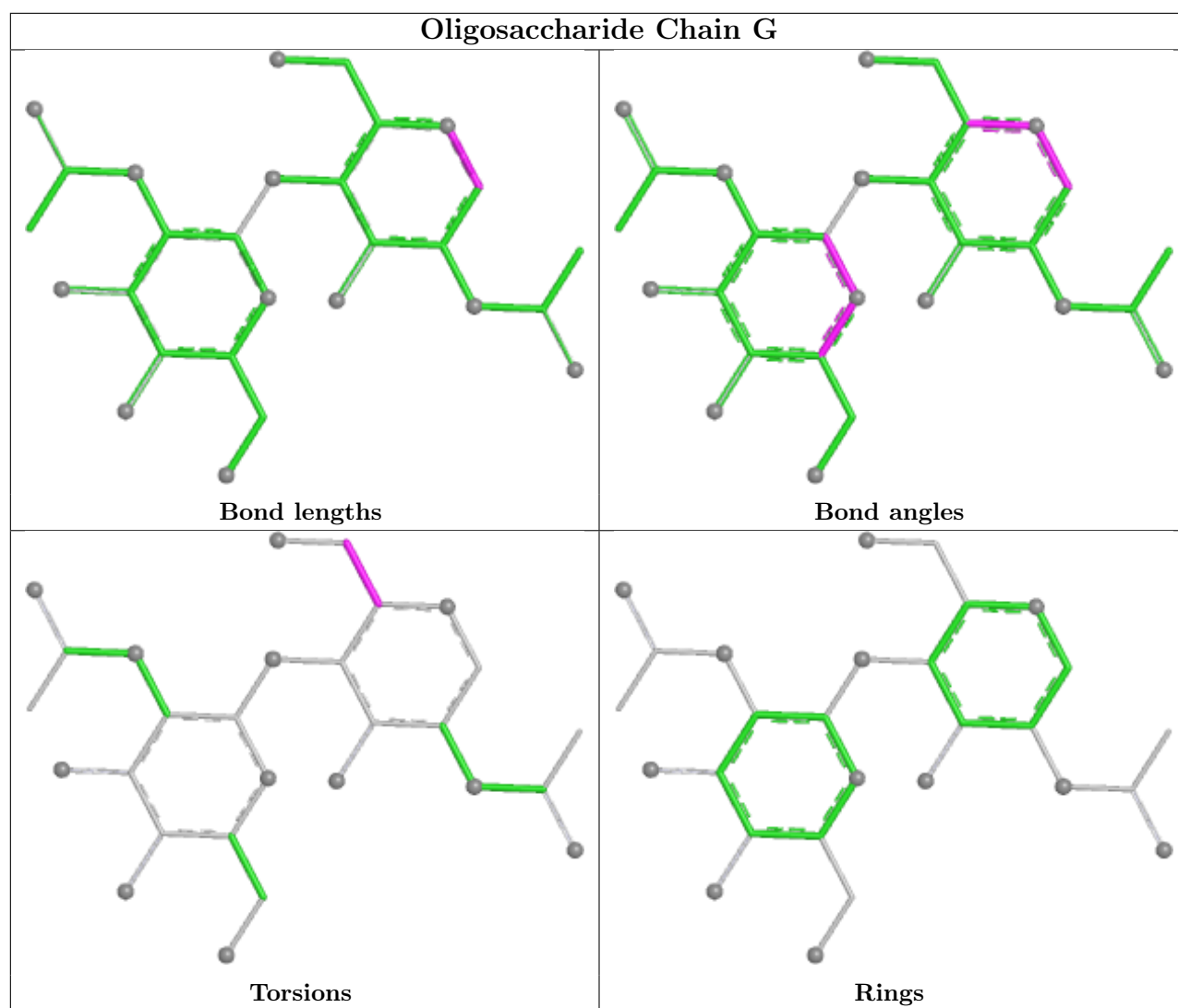


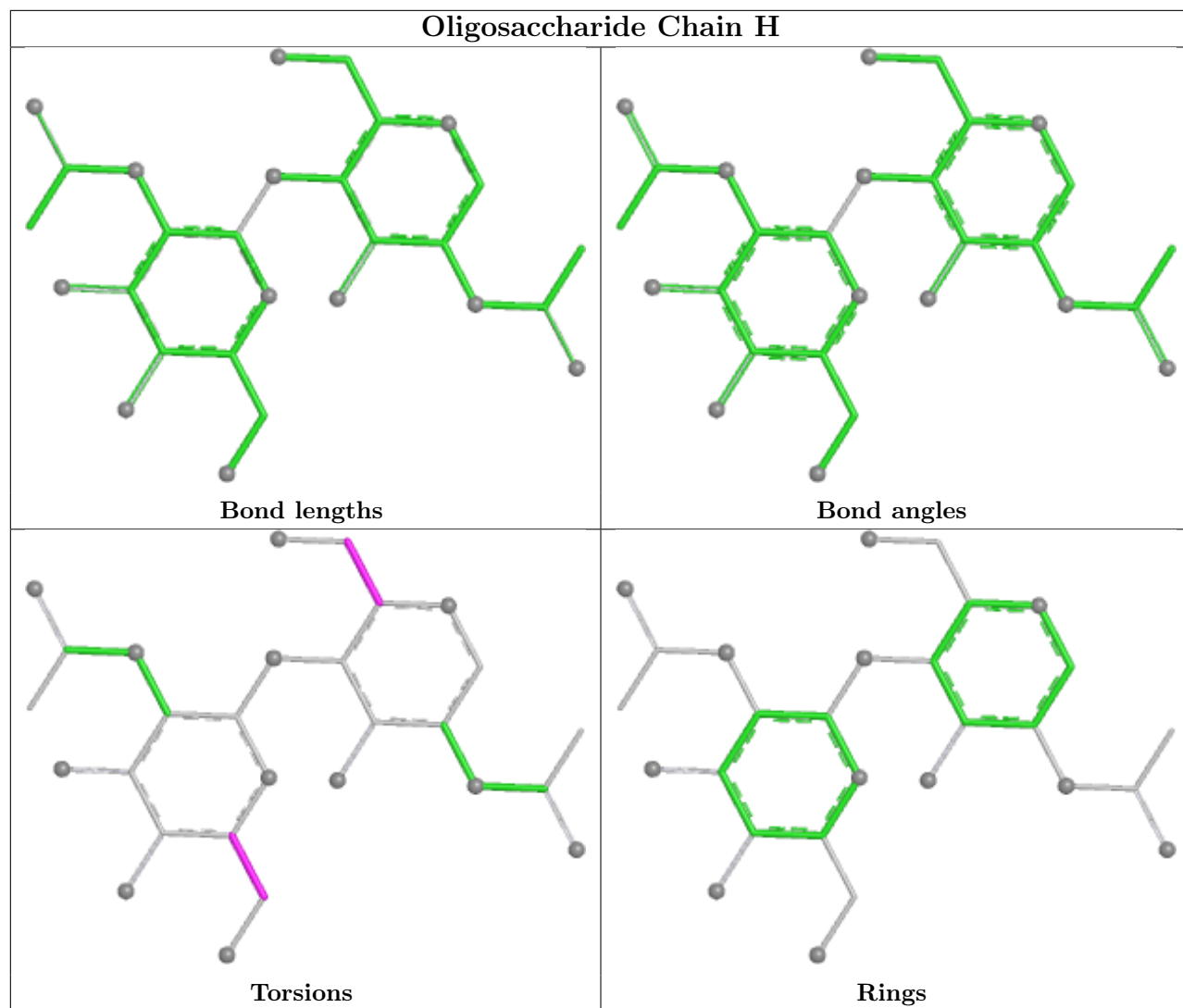


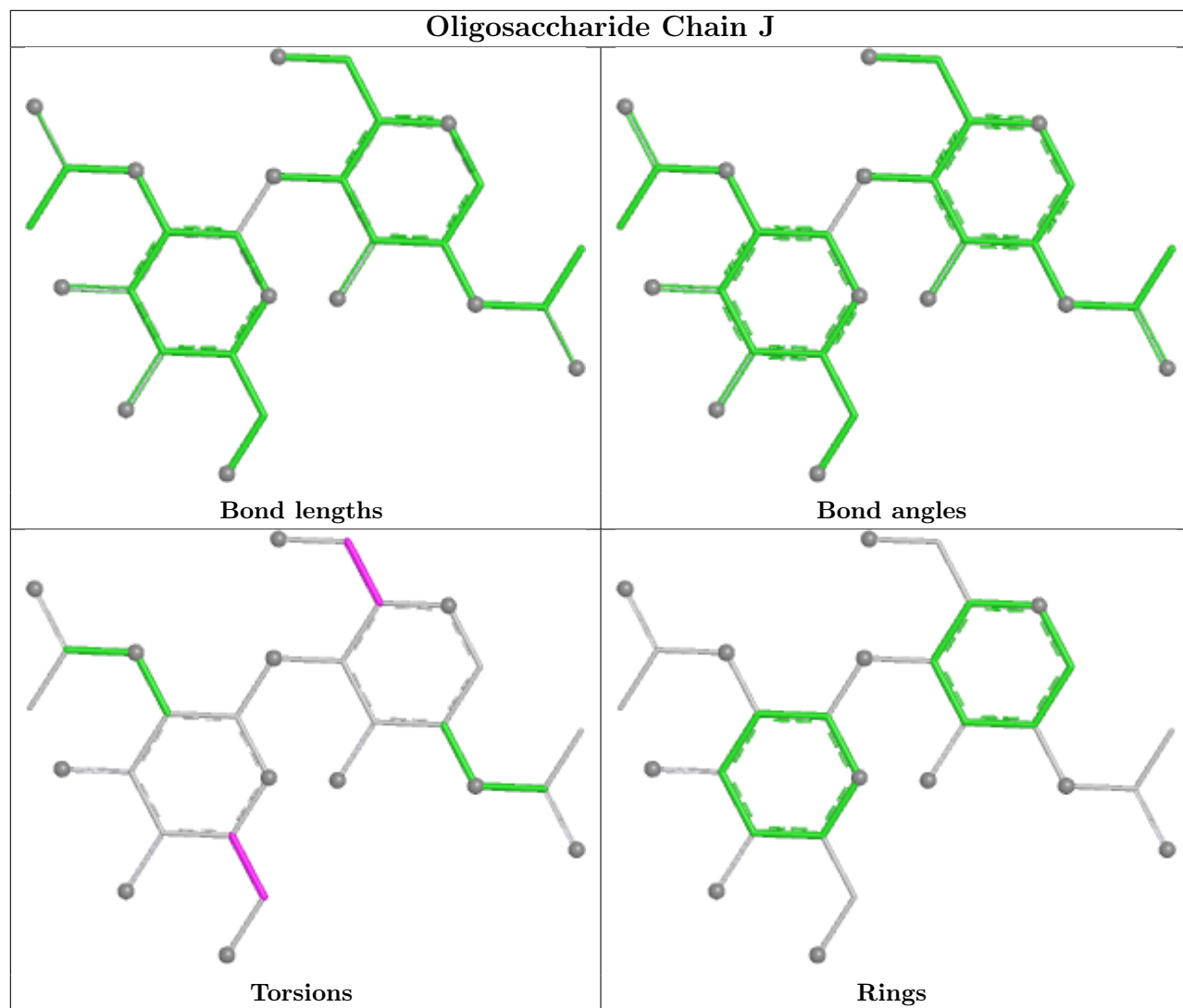


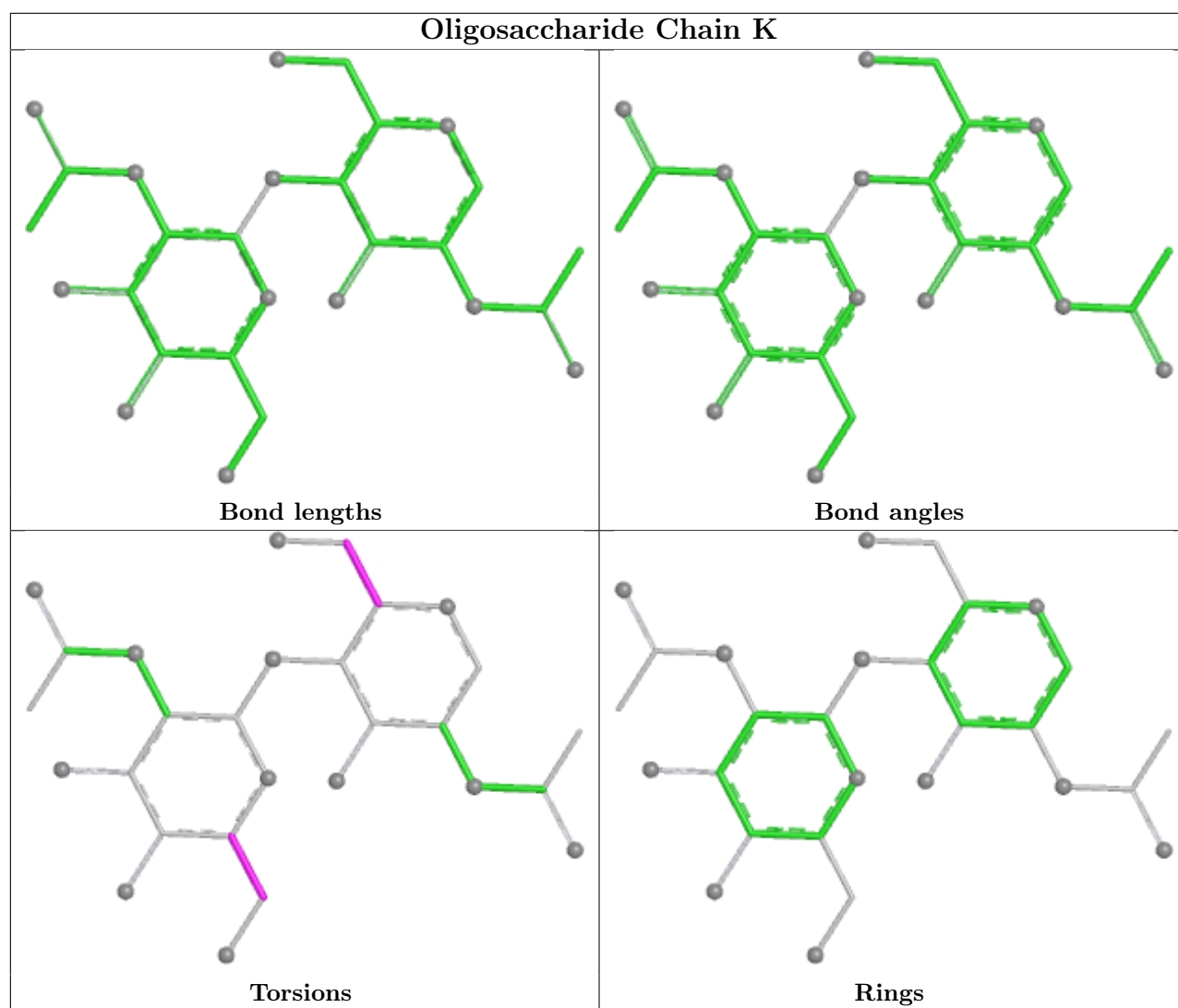


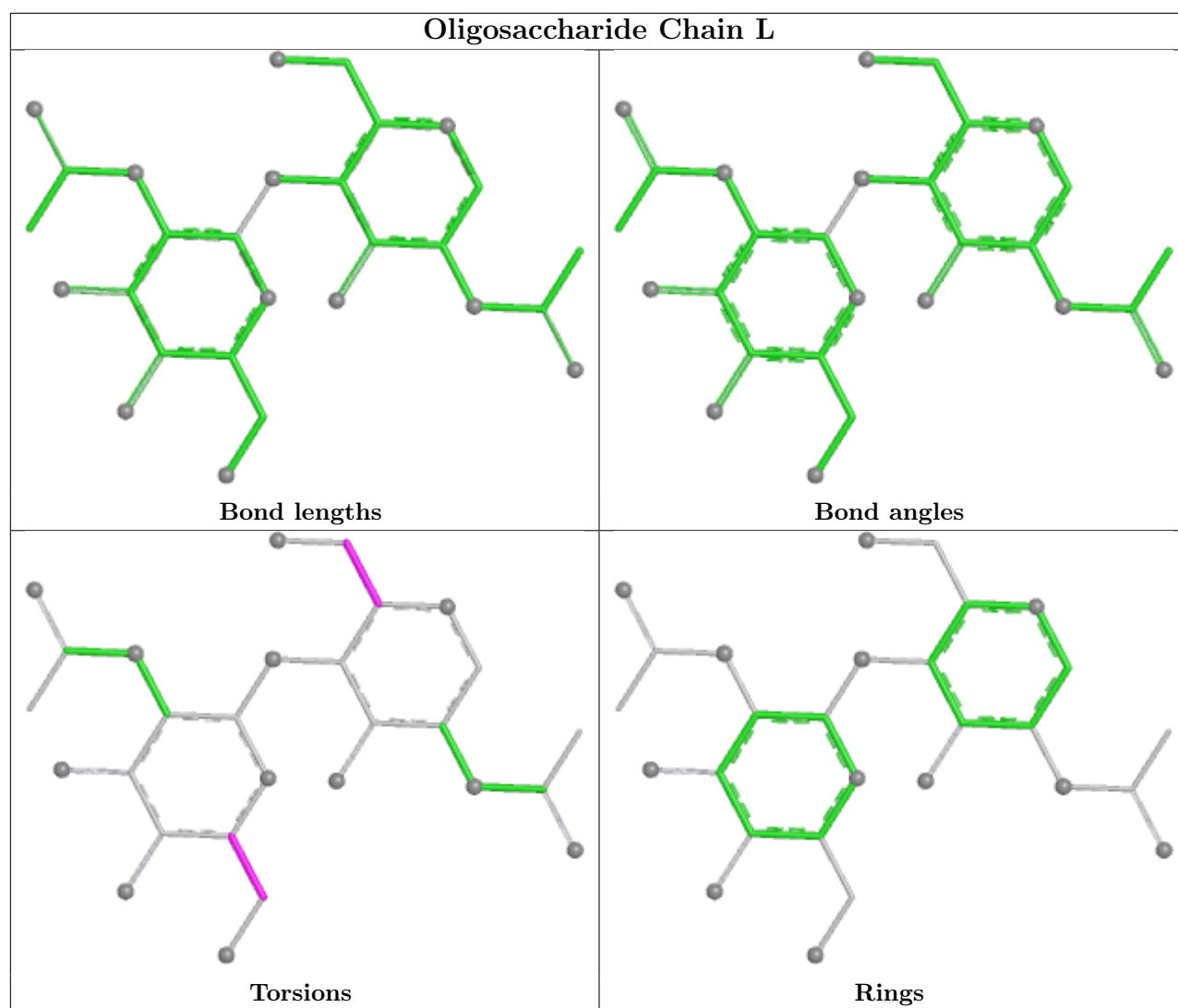


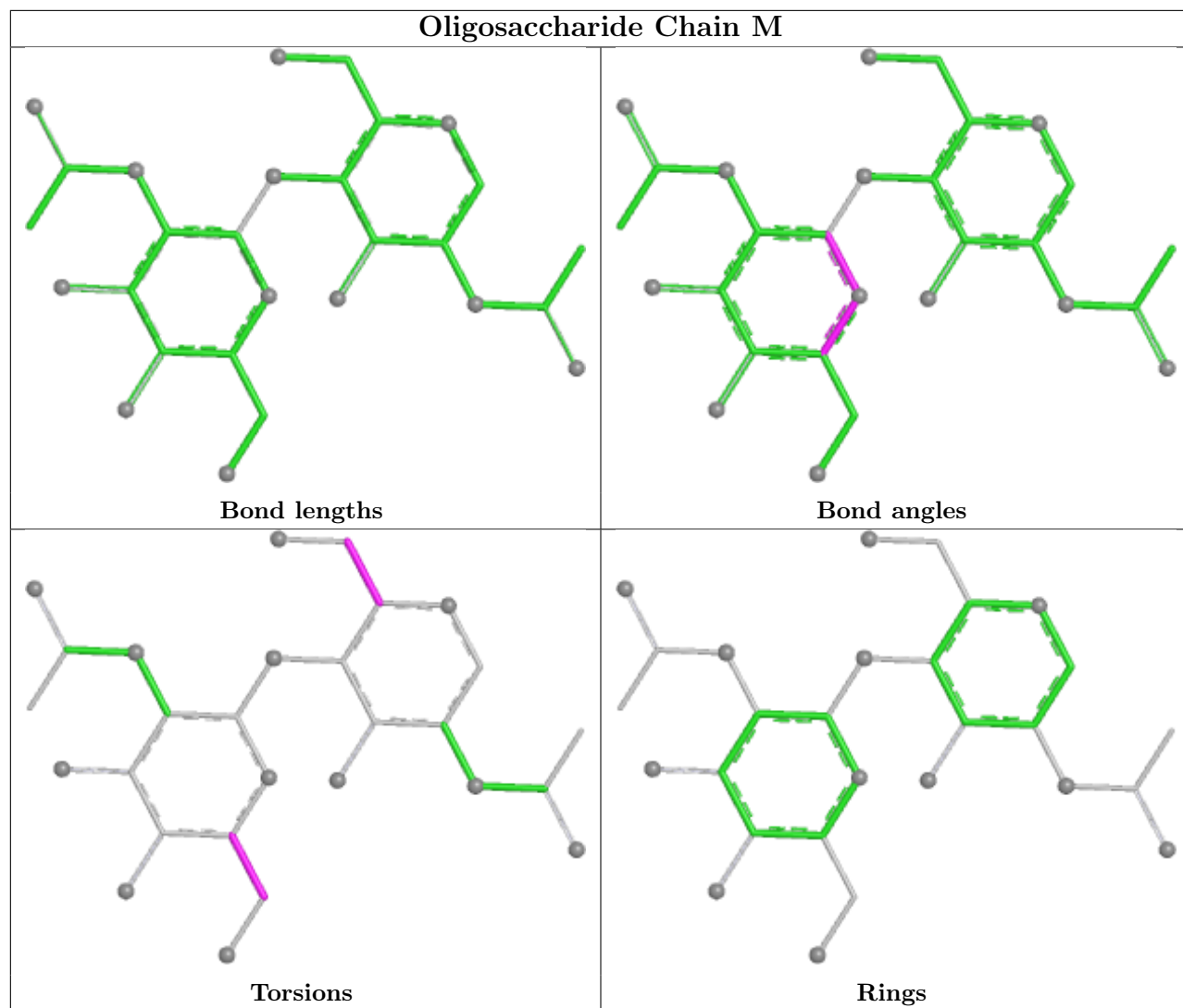


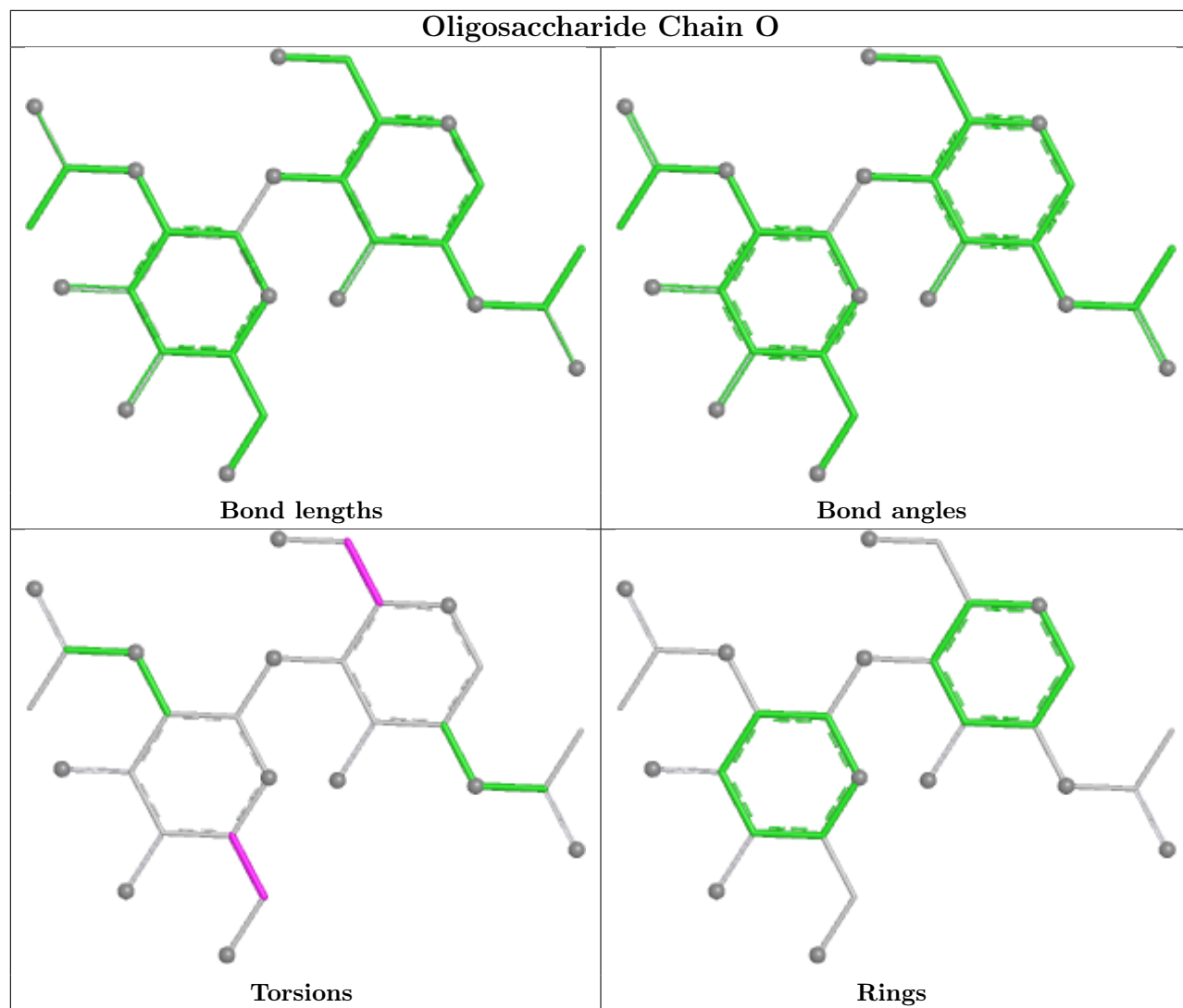


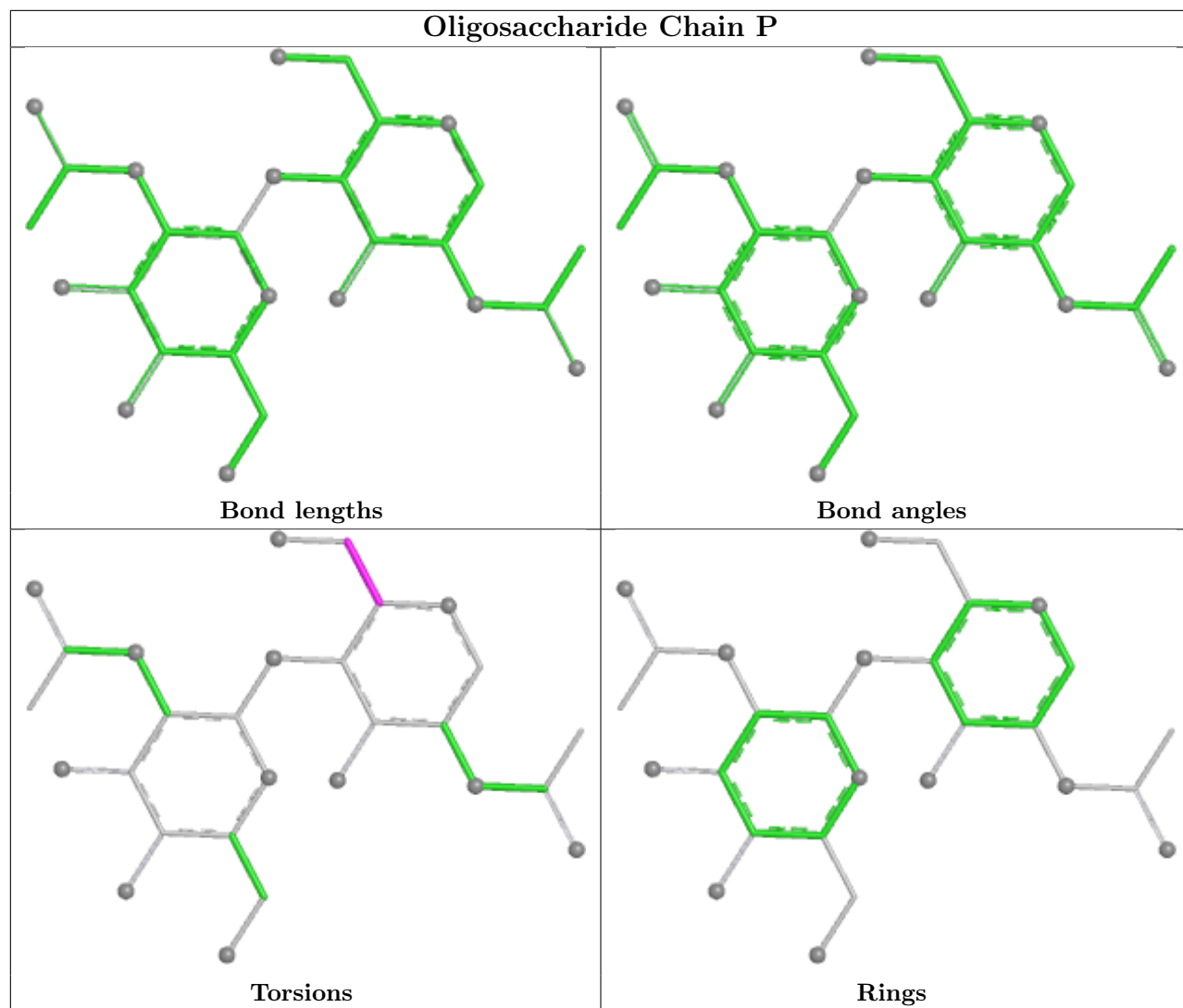


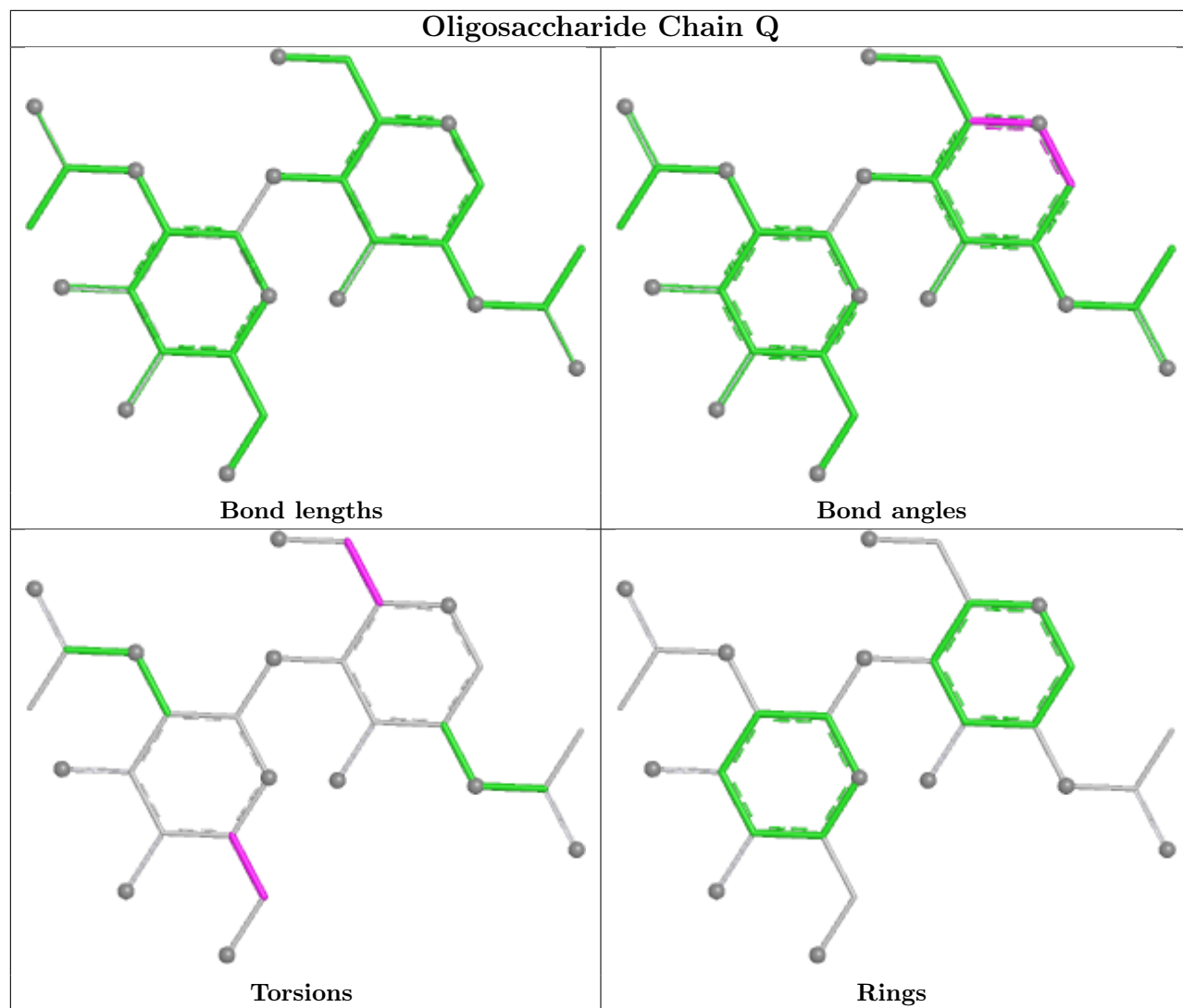


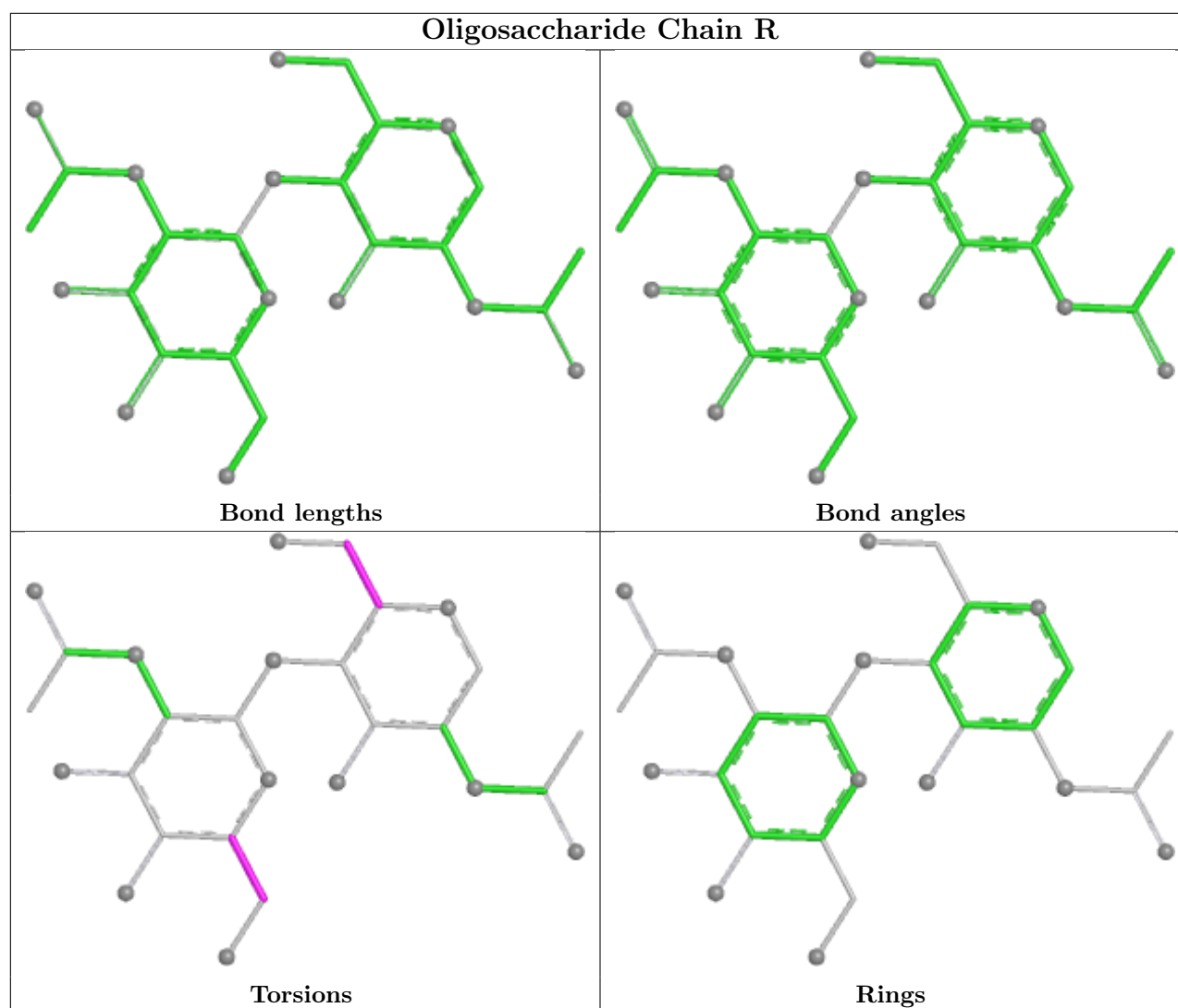












5.6 Ligand geometry [i](#)

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	B	2010	1	14,14,15	0.36	0	17,19,21	0.52	0
4	NAG	B	2016	1	14,14,15	0.28	0	17,19,21	0.59	0
4	NAG	B	2001	1	14,14,15	0.29	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2009	1	14,14,15	0.37	0	17,19,21	0.57	0
4	NAG	C	2006	1	14,14,15	0.39	0	17,19,21	0.49	0
4	NAG	C	2008	1	14,14,15	0.28	0	17,19,21	0.48	0
4	NAG	A	2006	1	14,14,15	0.48	0	17,19,21	0.43	0
4	NAG	B	2005	1	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	B	2011	1	14,14,15	0.41	0	17,19,21	0.57	0
4	NAG	B	2014	1	14,14,15	0.40	0	17,19,21	0.47	0
4	NAG	A	2003	1	14,14,15	0.68	0	17,19,21	0.49	0
4	NAG	B	2003	1	14,14,15	0.56	0	17,19,21	0.45	0
4	NAG	C	2012	1	14,14,15	0.31	0	17,19,21	0.46	0
4	NAG	A	2014	1	14,14,15	0.49	0	17,19,21	0.53	0
4	NAG	B	2015	1	14,14,15	0.42	0	17,19,21	0.68	1 (5%)
4	NAG	C	2002	1	14,14,15	0.46	0	17,19,21	0.59	0
4	NAG	C	2001	1	14,14,15	0.56	0	17,19,21	0.74	1 (5%)
4	NAG	B	2008	1	14,14,15	0.44	0	17,19,21	0.52	0
4	NAG	C	2007	1	14,14,15	0.38	0	17,19,21	0.50	0
4	NAG	C	2013	1	14,14,15	0.38	0	17,19,21	0.48	0
4	NAG	A	2007	1	14,14,15	0.37	0	17,19,21	0.48	0
4	NAG	B	2009	1	14,14,15	0.28	0	17,19,21	0.49	0
4	NAG	B	2004	1	14,14,15	0.40	0	17,19,21	0.55	0
4	NAG	B	2006	1	14,14,15	0.51	0	17,19,21	0.54	0
4	NAG	C	2009	1	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
4	NAG	A	2010	1	14,14,15	0.54	0	17,19,21	0.47	0
4	NAG	B	2013	1	14,14,15	0.46	0	17,19,21	0.44	0
4	NAG	A	2002	1	14,14,15	0.56	0	17,19,21	0.52	0
4	NAG	C	2014	1	14,14,15	0.33	0	17,19,21	0.37	0
4	NAG	A	2001	1	14,14,15	0.33	0	17,19,21	0.66	1 (5%)
4	NAG	A	2012	1	14,14,15	0.24	0	17,19,21	0.56	0
4	NAG	C	2005	1	14,14,15	0.37	0	17,19,21	0.51	0
4	NAG	B	2002	1	14,14,15	0.35	0	17,19,21	0.47	0
4	NAG	C	2003	1	14,14,15	0.55	0	17,19,21	0.60	0
4	NAG	C	2010	1	14,14,15	0.41	0	17,19,21	0.65	1 (5%)
4	NAG	A	2005	1	14,14,15	0.36	0	17,19,21	0.41	0
4	NAG	A	2016	1	14,14,15	0.51	0	17,19,21	0.56	0
4	NAG	C	2015	1	14,14,15	0.30	0	17,19,21	0.49	0
4	NAG	C	2011	1	14,14,15	0.40	0	17,19,21	0.56	0
4	NAG	A	2004	1	14,14,15	0.40	0	17,19,21	0.62	1 (5%)
4	NAG	C	2017	1	14,14,15	0.55	0	17,19,21	0.57	0
4	NAG	B	2017	1	14,14,15	0.43	0	17,19,21	0.57	0
4	NAG	A	2011	1	14,14,15	0.28	0	17,19,21	0.47	0
4	NAG	A	2017	1	14,14,15	0.44	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	2007	1	14,14,15	0.47	0	17,19,21	0.61	1 (5%)
4	NAG	C	2016	1	14,14,15	0.32	0	17,19,21	0.63	1 (5%)
4	NAG	A	2015	1	14,14,15	0.45	0	17,19,21	0.47	0
4	NAG	B	2012	1	14,14,15	0.28	0	17,19,21	0.67	1 (5%)
4	NAG	A	2013	1	14,14,15	0.55	0	17,19,21	0.35	0
4	NAG	A	2008	1	14,14,15	0.33	0	17,19,21	0.50	0
4	NAG	C	2004	1	14,14,15	0.42	0	17,19,21	0.63	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	2010	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2016	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2008	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	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2011	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2012	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2015	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2001	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	2007	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2013	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	2009	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	2006	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	2010	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2013	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2012	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2005	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	3/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2010	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2016	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	2011	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2017	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2017	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2011	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2017	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2007	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2016	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2015	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2012	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2013	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2001	NAG	C1-O5-C5	2.60	115.68	112.19
4	C	2009	NAG	C1-O5-C5	2.33	115.31	112.19
4	C	2010	NAG	C1-O5-C5	2.30	115.26	112.19
4	B	2015	NAG	C1-O5-C5	2.28	115.24	112.19
4	A	2001	NAG	C1-O5-C5	2.22	115.16	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2004	NAG	C1-O5-C5	2.21	115.15	112.19
4	A	2004	NAG	C1-O5-C5	2.13	115.05	112.19
4	C	2016	NAG	C1-O5-C5	2.10	115.00	112.19
4	B	2007	NAG	C1-O5-C5	2.05	114.94	112.19
4	B	2012	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2006	NAG	O5-C5-C6-O6
4	C	2002	NAG	O5-C5-C6-O6
4	B	2014	NAG	C4-C5-C6-O6
4	A	2017	NAG	O5-C5-C6-O6
4	B	2008	NAG	O5-C5-C6-O6
4	A	2008	NAG	O5-C5-C6-O6
4	B	2003	NAG	O5-C5-C6-O6
4	B	2010	NAG	O5-C5-C6-O6
4	B	2016	NAG	O5-C5-C6-O6
4	A	2015	NAG	O5-C5-C6-O6
4	C	2001	NAG	O5-C5-C6-O6
4	A	2013	NAG	O5-C5-C6-O6
4	C	2002	NAG	C4-C5-C6-O6
4	C	2013	NAG	C4-C5-C6-O6
4	A	2017	NAG	C4-C5-C6-O6
4	A	2001	NAG	O5-C5-C6-O6
4	B	2002	NAG	O5-C5-C6-O6
4	A	2003	NAG	O5-C5-C6-O6
4	B	2006	NAG	C4-C5-C6-O6
4	A	2008	NAG	C4-C5-C6-O6
4	C	2014	NAG	O5-C5-C6-O6
4	B	2014	NAG	O5-C5-C6-O6
4	B	2015	NAG	O5-C5-C6-O6
4	A	2003	NAG	C4-C5-C6-O6
4	C	2003	NAG	O5-C5-C6-O6
4	C	2004	NAG	O5-C5-C6-O6
4	C	2006	NAG	O5-C5-C6-O6
4	C	2010	NAG	O5-C5-C6-O6
4	A	2002	NAG	O5-C5-C6-O6
4	A	2005	NAG	O5-C5-C6-O6
4	A	2014	NAG	O5-C5-C6-O6
4	A	2001	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	2005	NAG	C4-C5-C6-O6
4	B	2010	NAG	C4-C5-C6-O6
4	C	2017	NAG	O5-C5-C6-O6
4	B	2003	NAG	C4-C5-C6-O6
4	B	2015	NAG	C4-C5-C6-O6
4	B	2016	NAG	C4-C5-C6-O6
4	C	2010	NAG	C4-C5-C6-O6
4	C	2014	NAG	C4-C5-C6-O6
4	A	2002	NAG	C4-C5-C6-O6
4	A	2014	NAG	C4-C5-C6-O6
4	C	2009	NAG	O5-C5-C6-O6
4	A	2007	NAG	O5-C5-C6-O6
4	B	2008	NAG	C4-C5-C6-O6
4	C	2004	NAG	C4-C5-C6-O6
4	C	2001	NAG	C4-C5-C6-O6
4	B	2011	NAG	O5-C5-C6-O6
4	B	2017	NAG	O5-C5-C6-O6
4	A	2015	NAG	C4-C5-C6-O6
4	B	2002	NAG	C4-C5-C6-O6
4	C	2003	NAG	C4-C5-C6-O6
4	C	2009	NAG	C4-C5-C6-O6
4	C	2006	NAG	C4-C5-C6-O6
4	C	2013	NAG	O5-C5-C6-O6
4	A	2009	NAG	O5-C5-C6-O6
4	A	2013	NAG	C4-C5-C6-O6
4	C	2017	NAG	C4-C5-C6-O6
4	B	2012	NAG	C4-C5-C6-O6
4	B	2012	NAG	O5-C5-C6-O6
4	A	2006	NAG	C4-C5-C6-O6
4	A	2010	NAG	O5-C5-C6-O6
4	B	2001	NAG	C4-C5-C6-O6
4	B	2017	NAG	C4-C5-C6-O6
4	A	2006	NAG	O5-C5-C6-O6
4	A	2016	NAG	O5-C5-C6-O6
4	B	2011	NAG	C4-C5-C6-O6
4	B	2005	NAG	C4-C5-C6-O6
4	B	2005	NAG	O5-C5-C6-O6
4	A	2009	NAG	C4-C5-C6-O6
4	B	2001	NAG	O5-C5-C6-O6
4	A	2007	NAG	C4-C5-C6-O6
4	B	2002	NAG	C1-C2-N2-C7
4	A	2016	NAG	C1-C2-N2-C7

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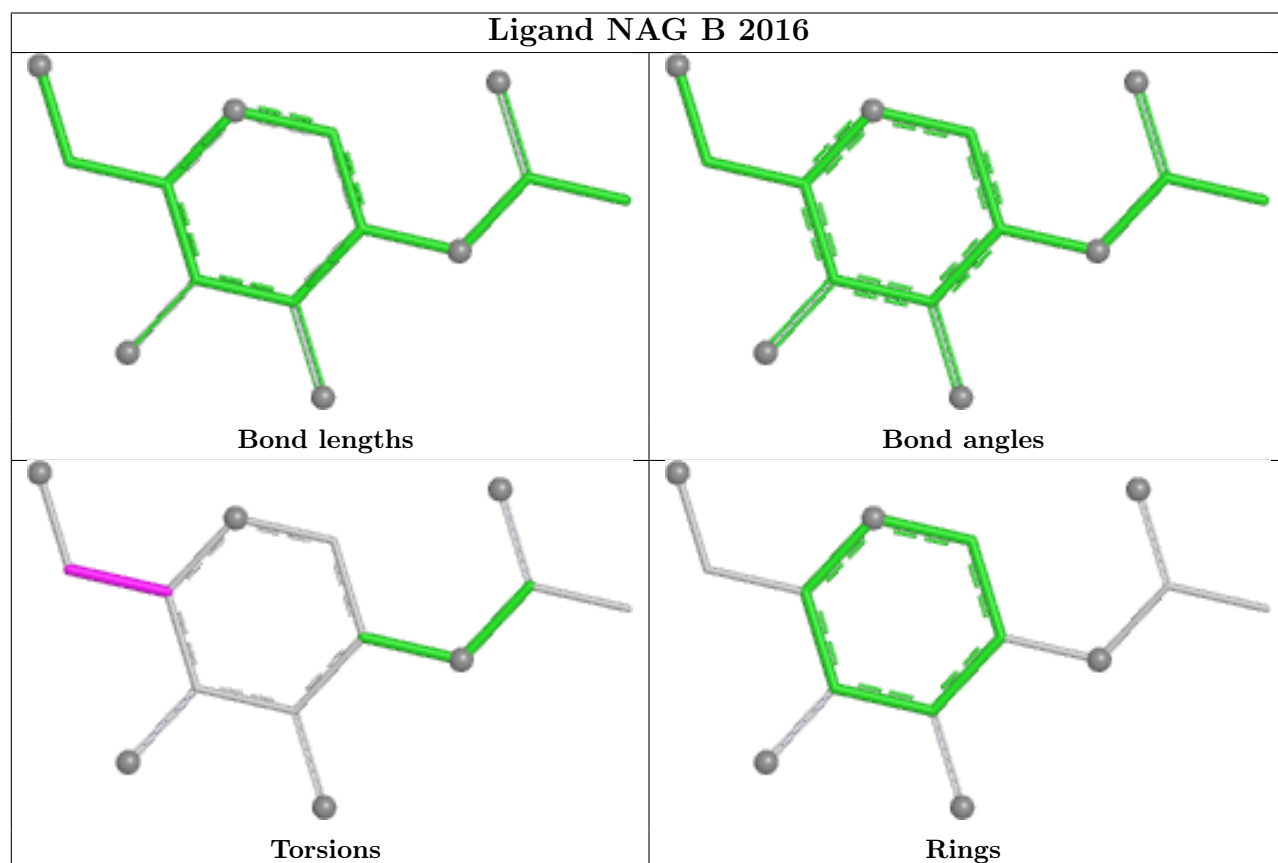
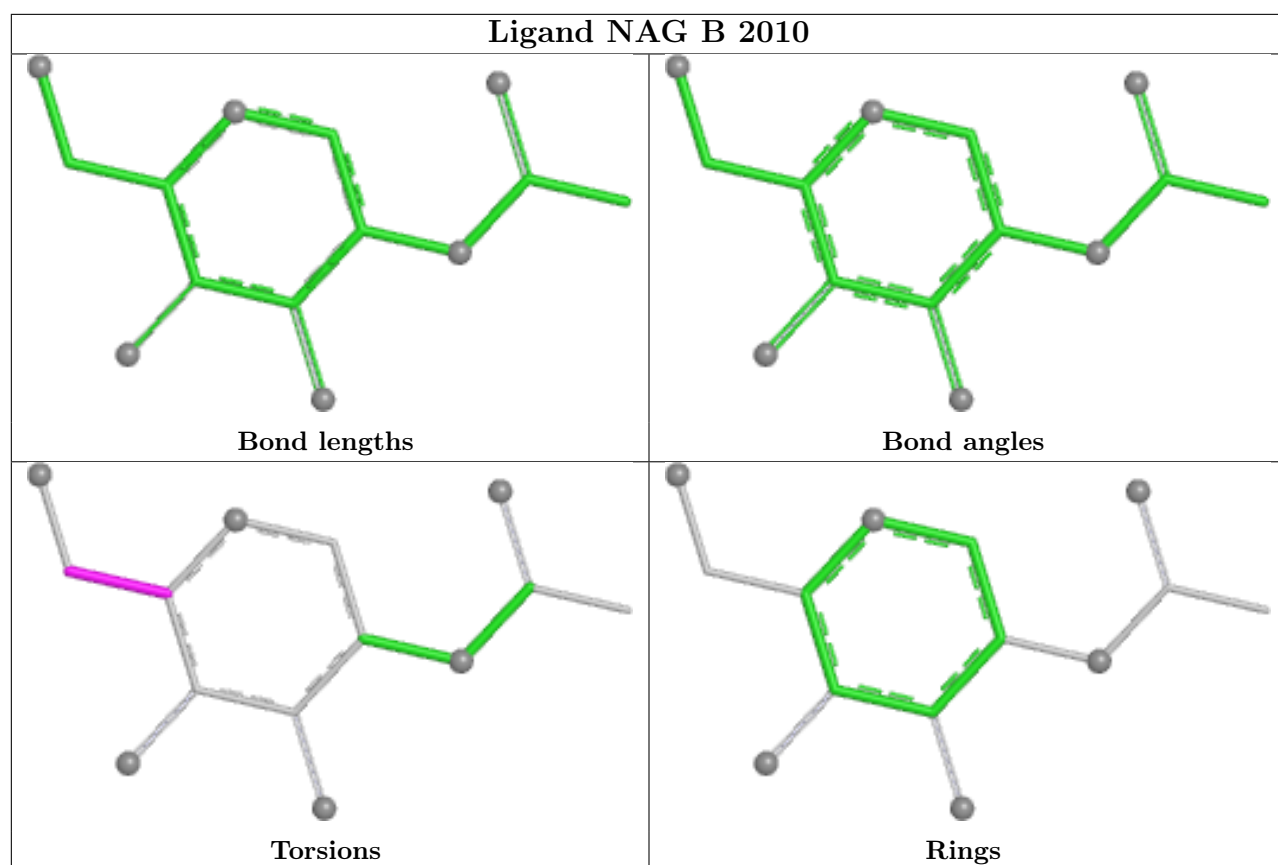
Mol	Chain	Res	Type	Atoms
4	A	2004	NAG	C4-C5-C6-O6

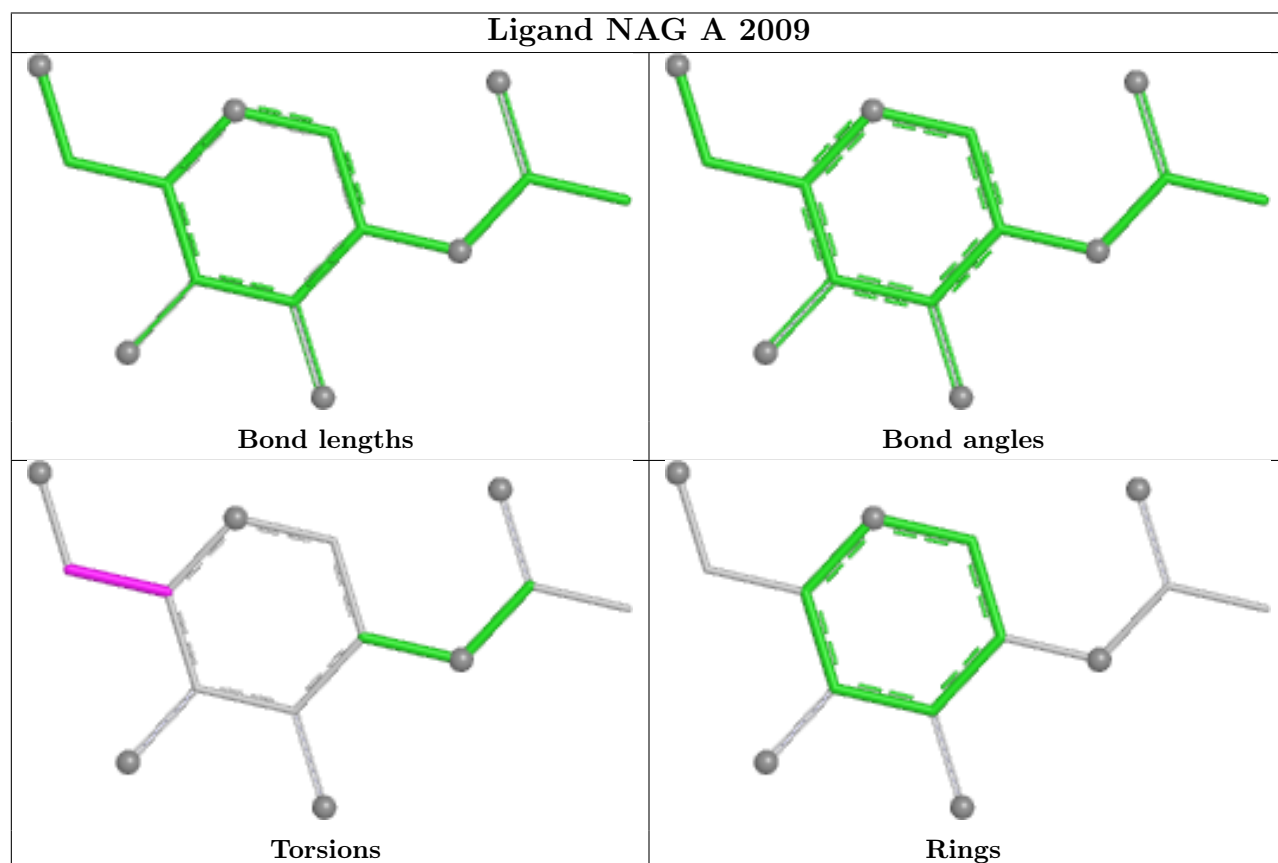
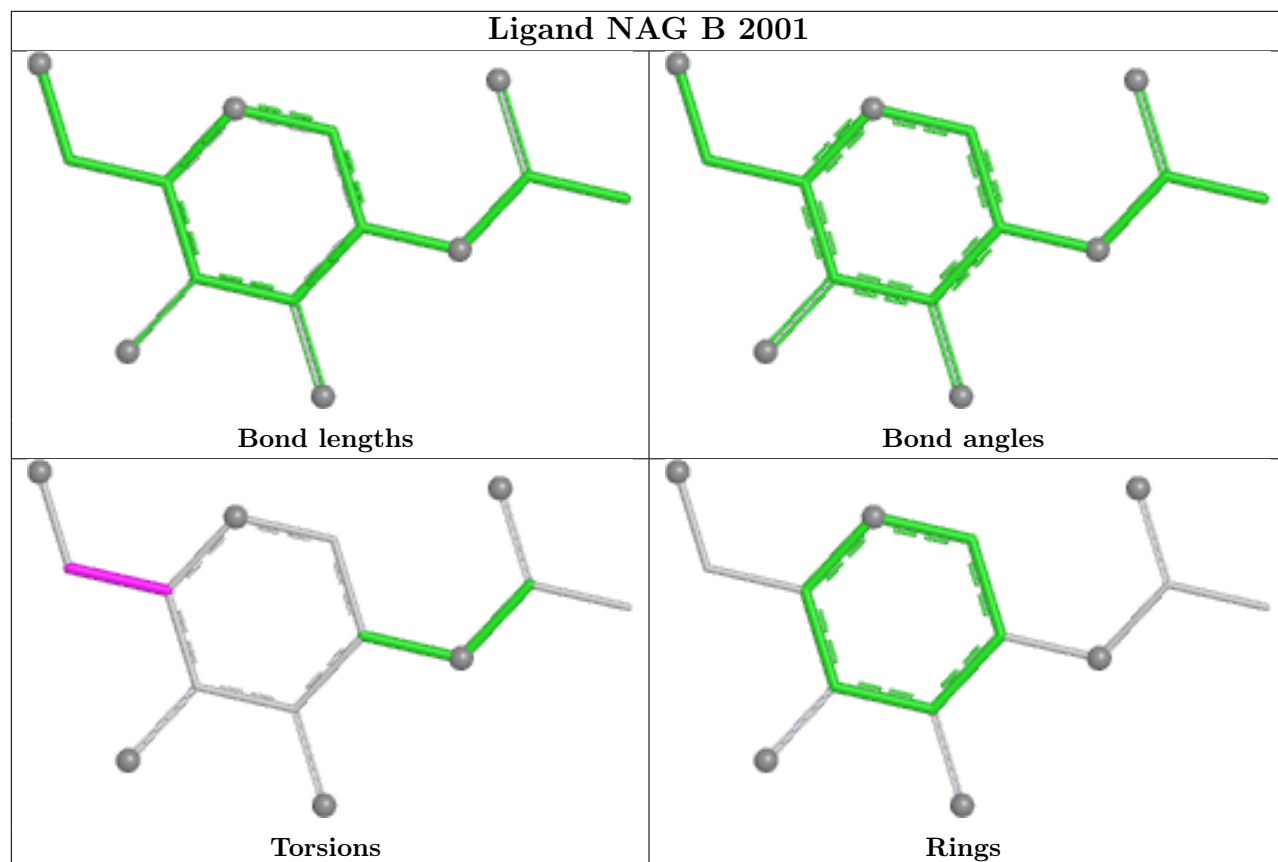
There are no ring outliers.

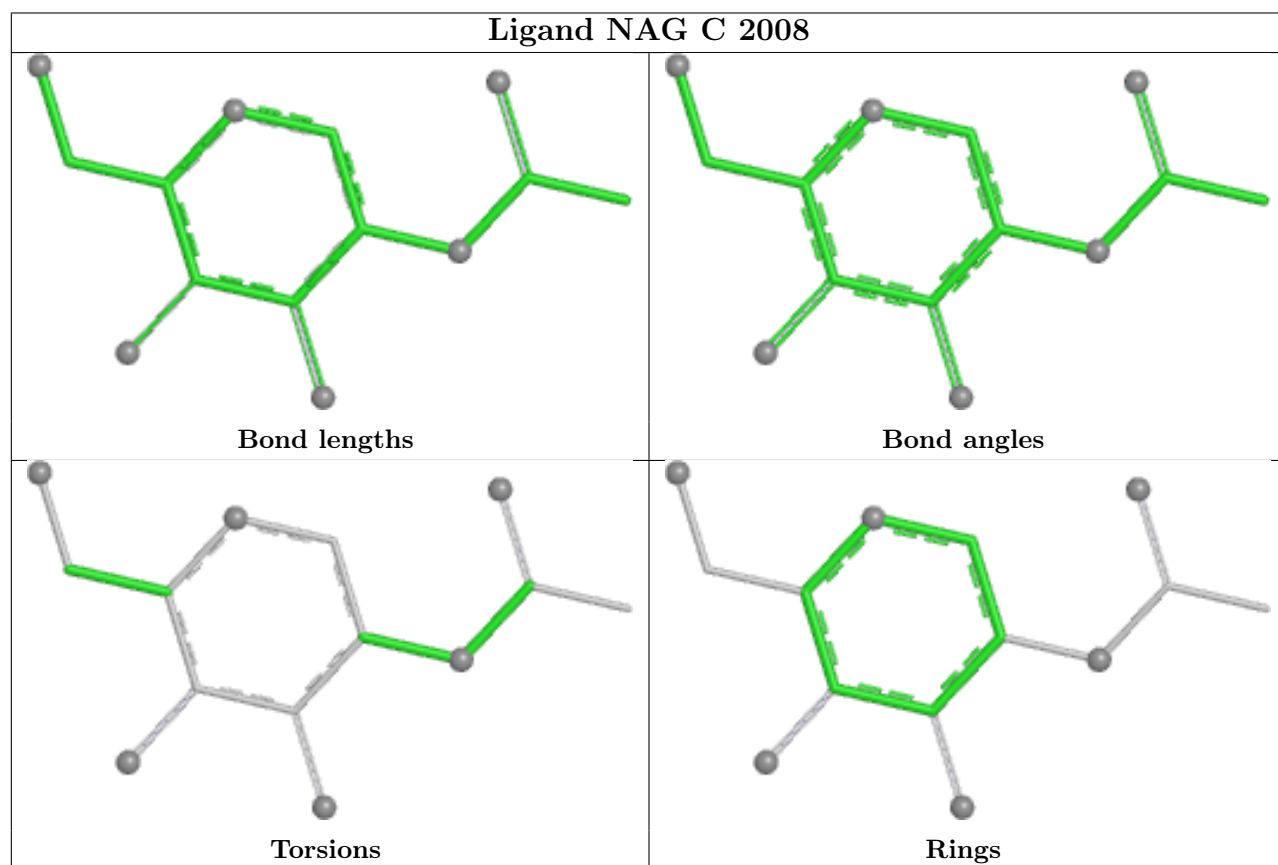
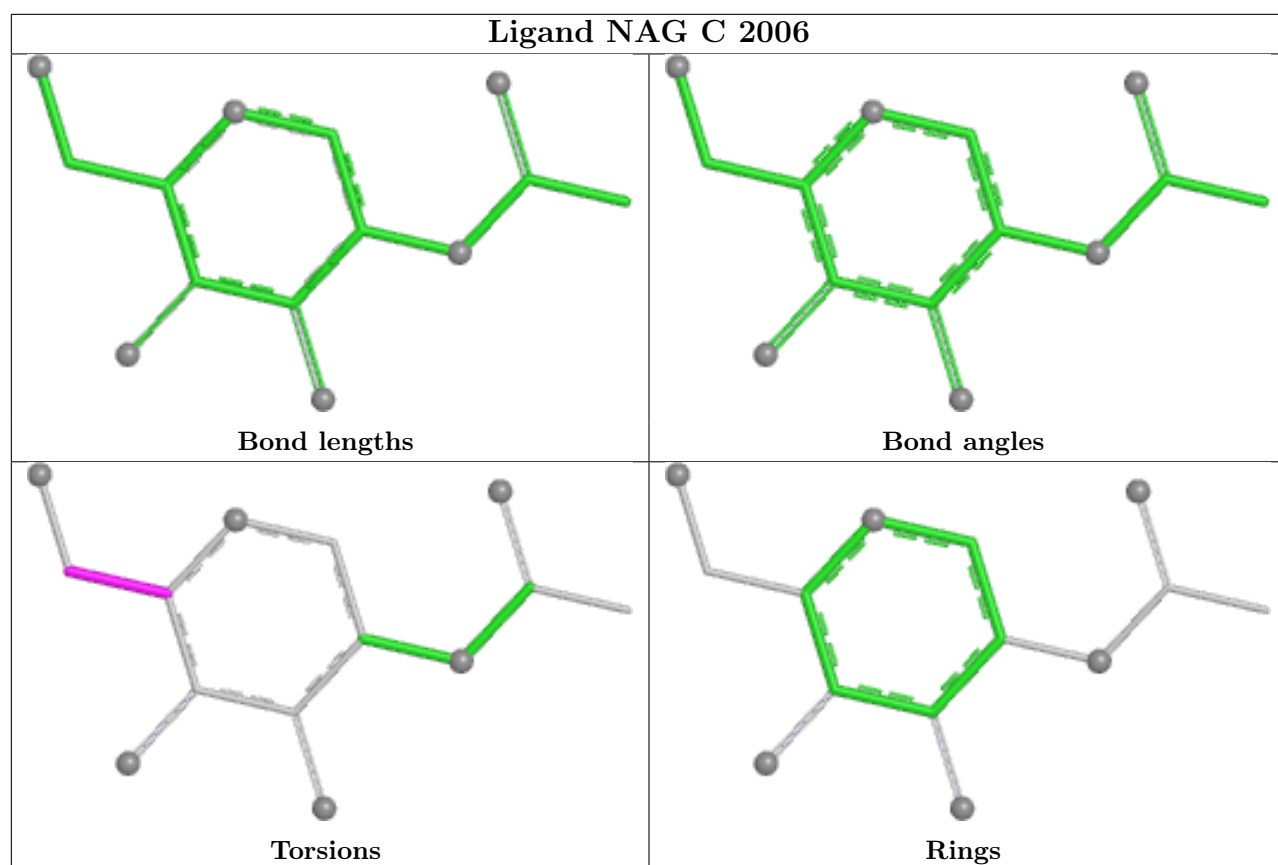
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2014	NAG	1	0
4	A	2012	NAG	2	0

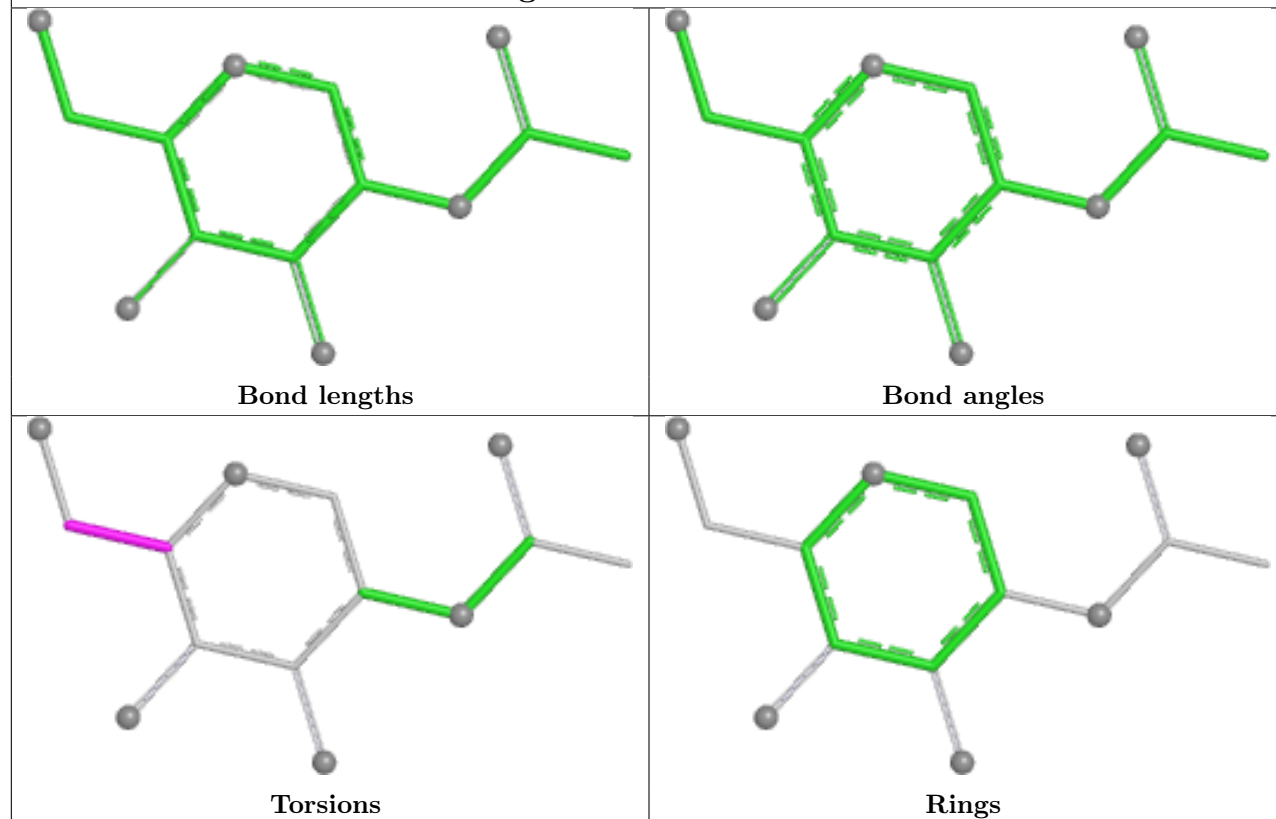
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



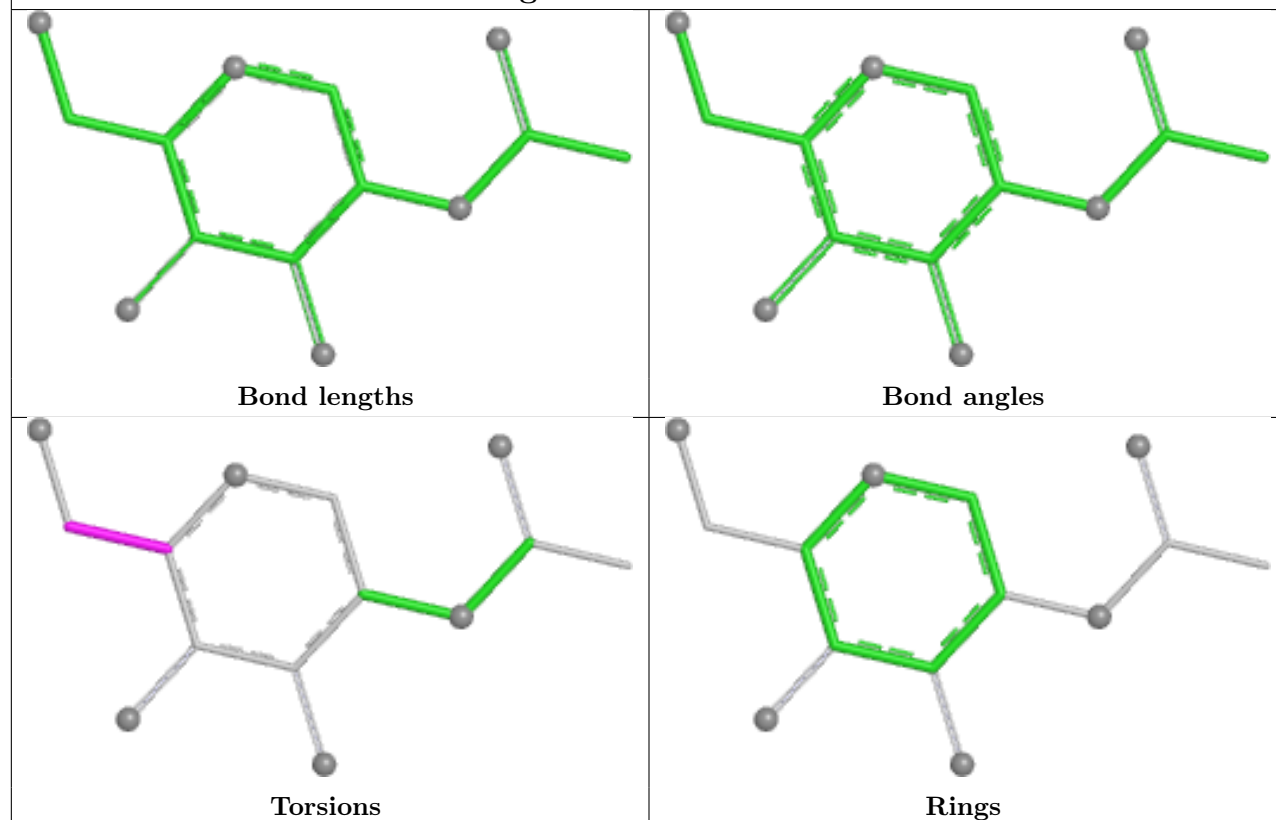




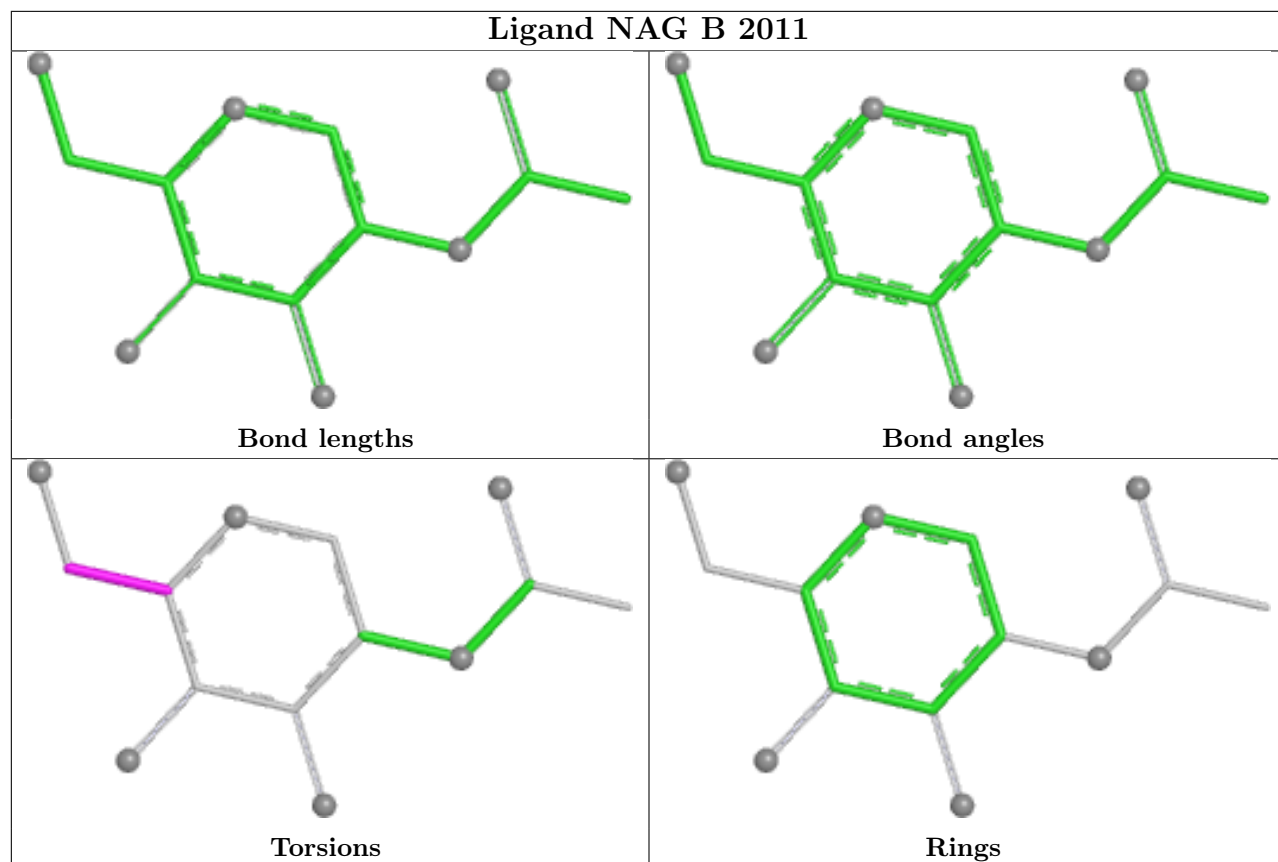
Ligand NAG A 2006



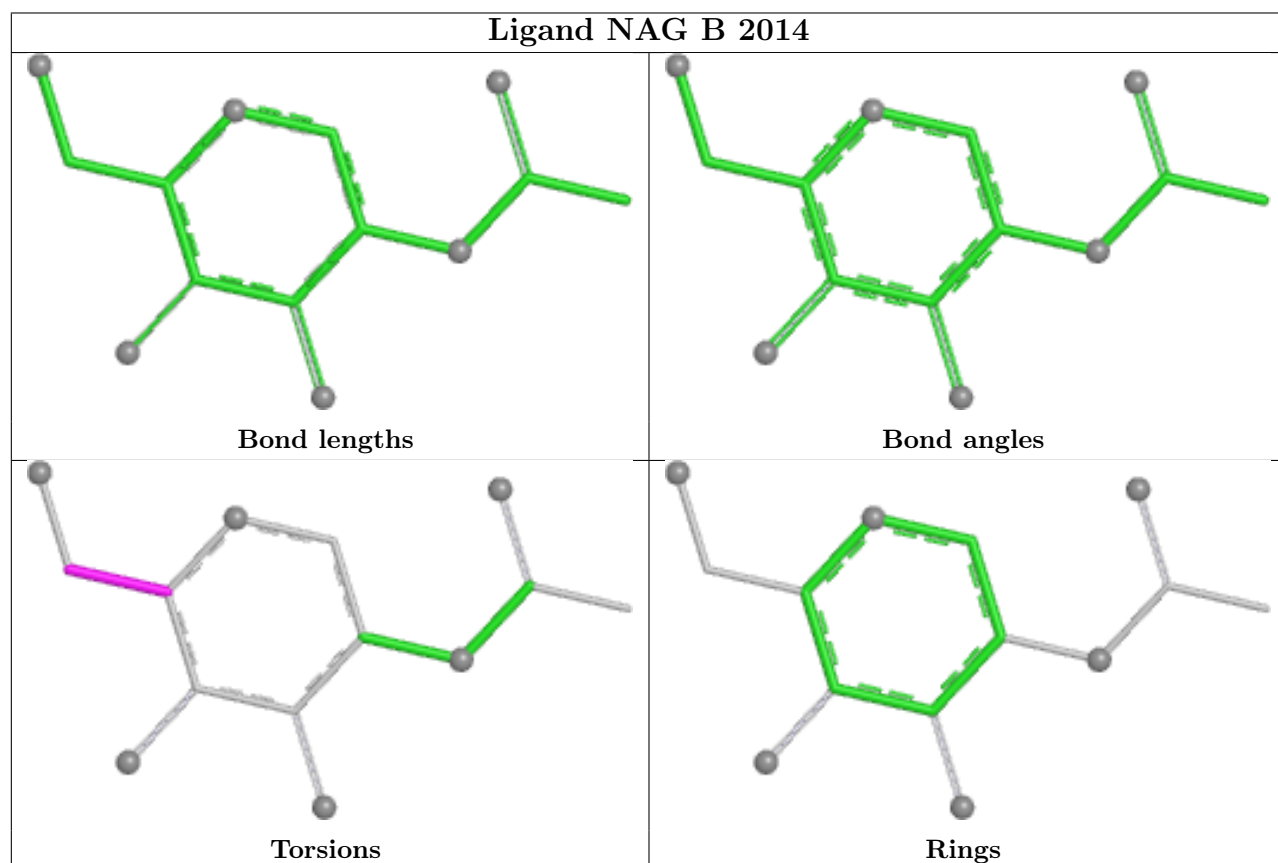
Ligand NAG B 2005



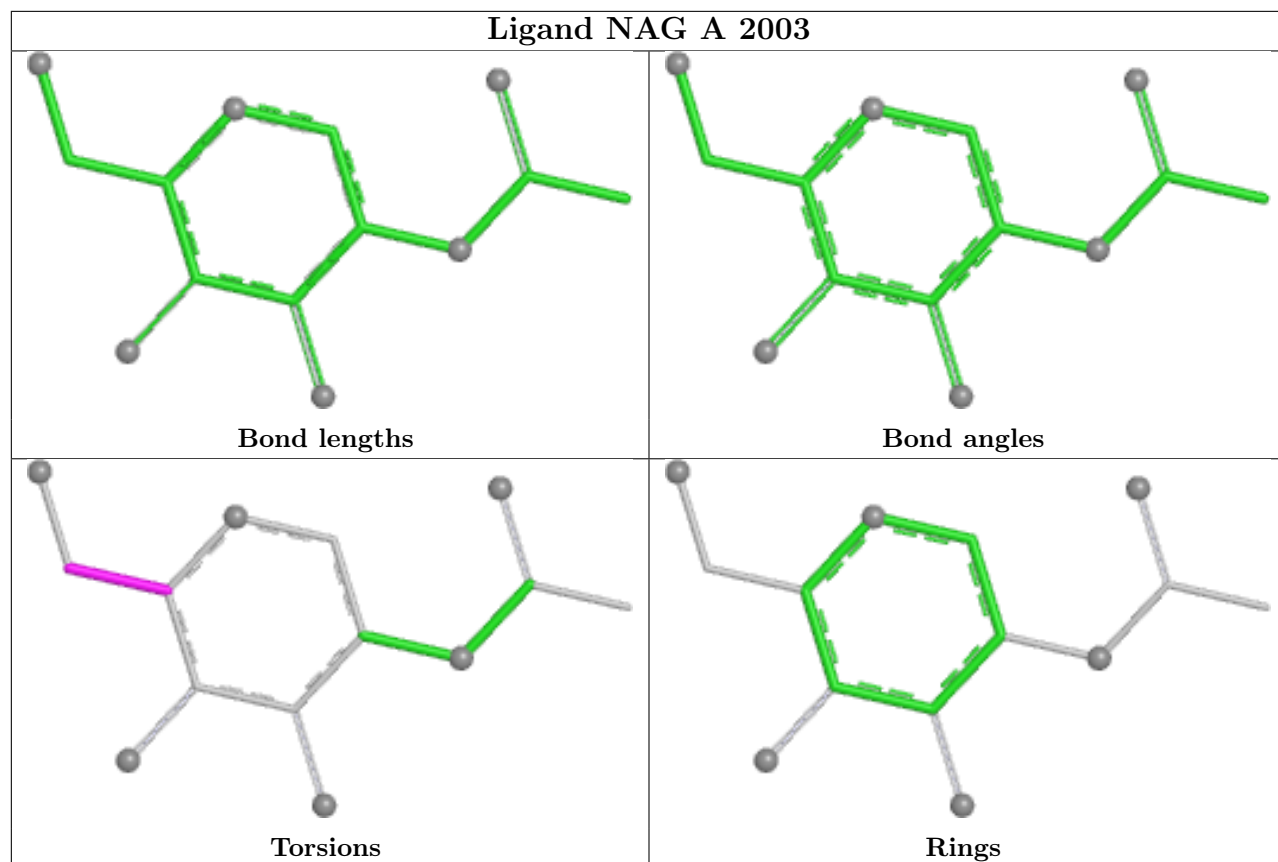
Ligand NAG B 2011



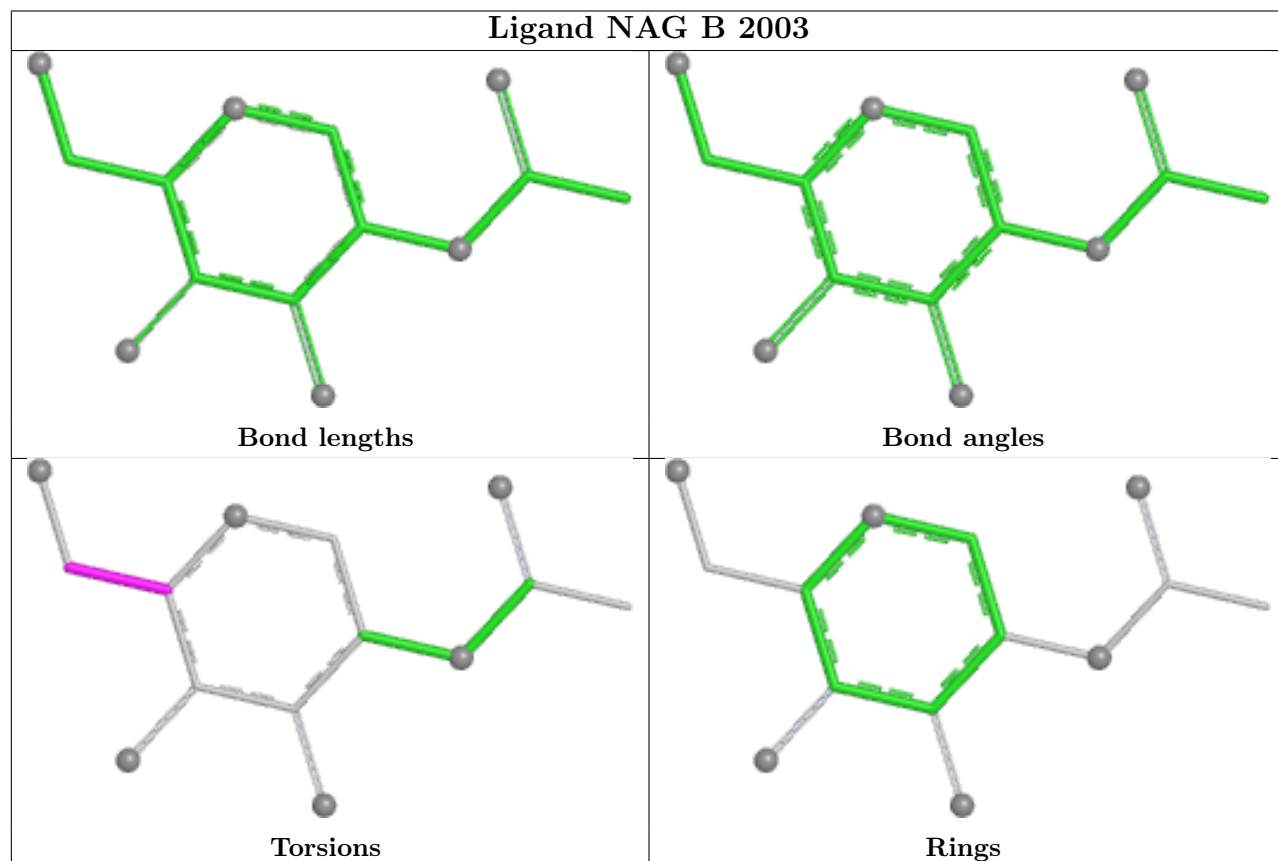
Ligand NAG B 2014

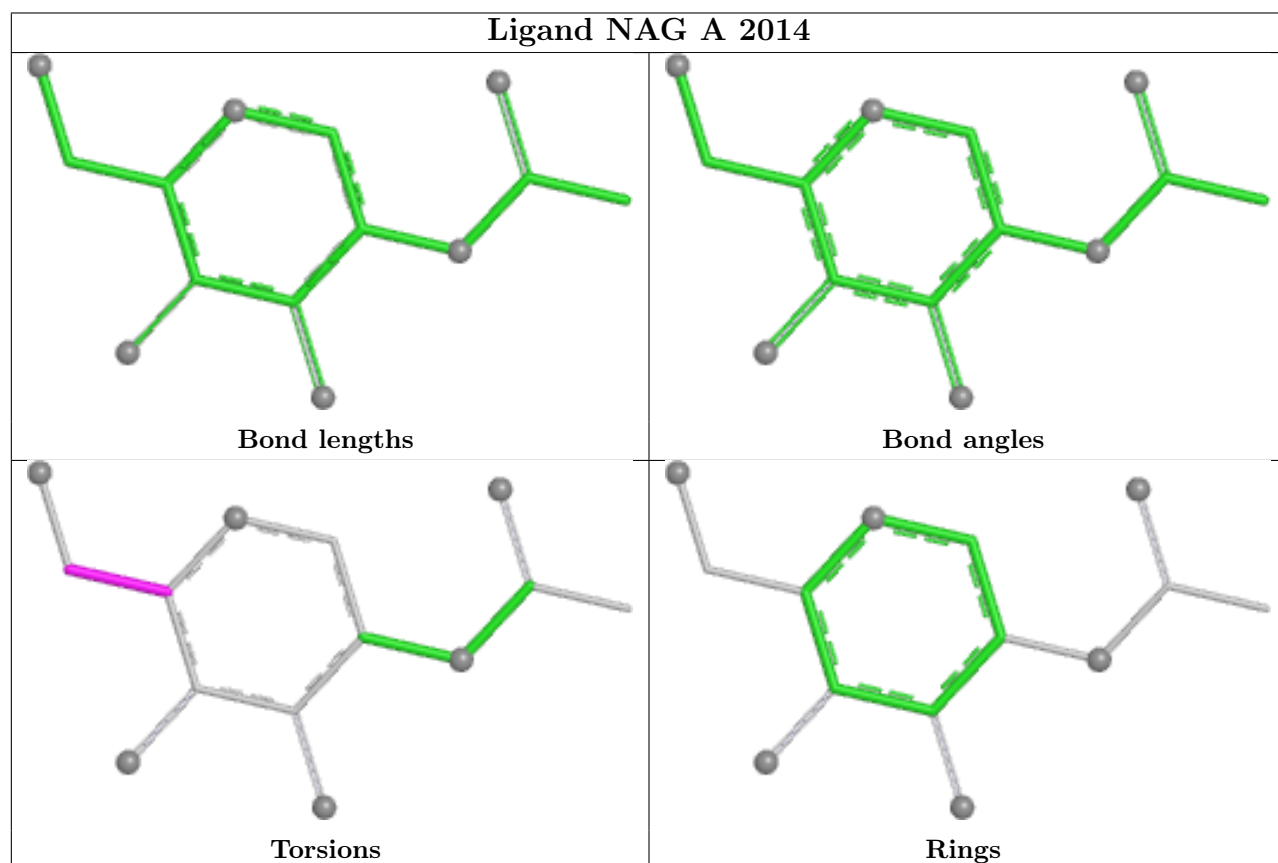
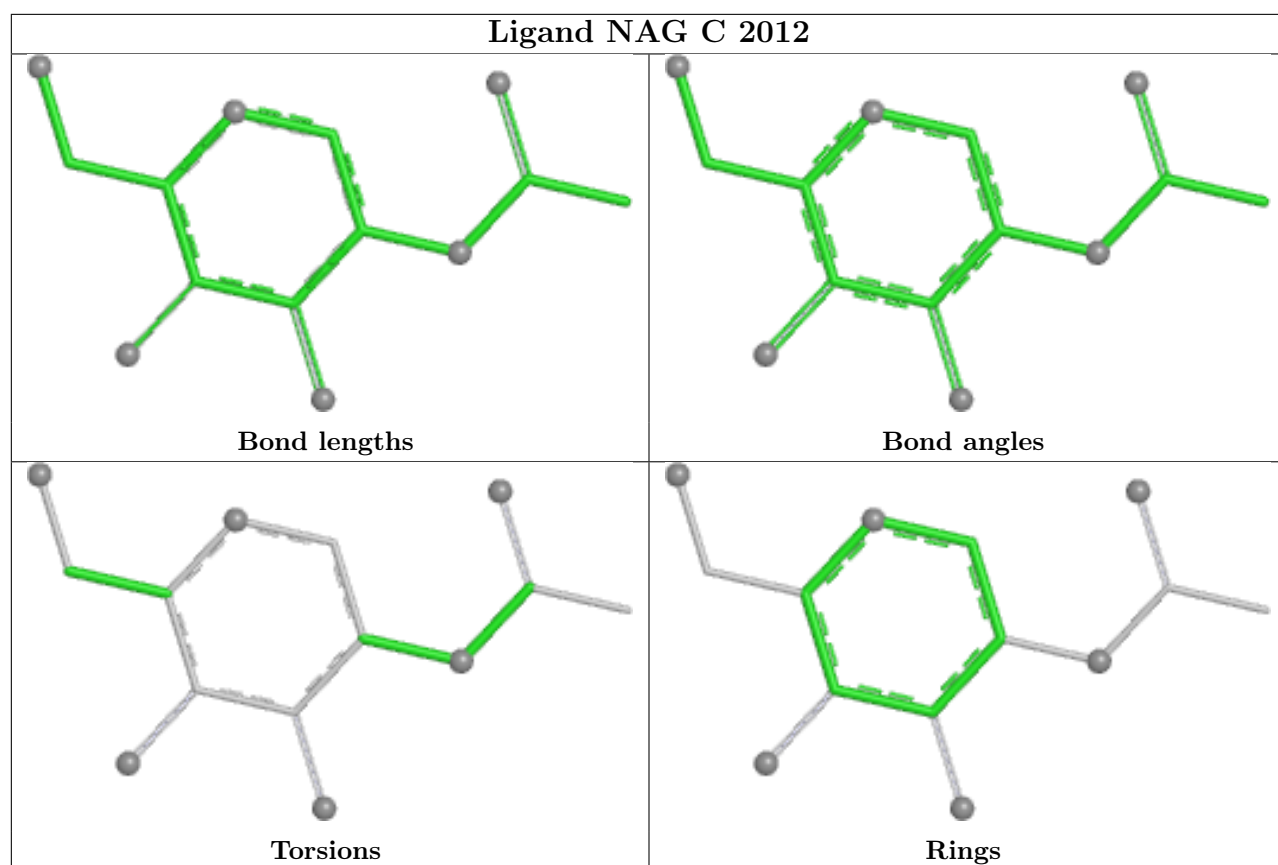


Ligand NAG A 2003

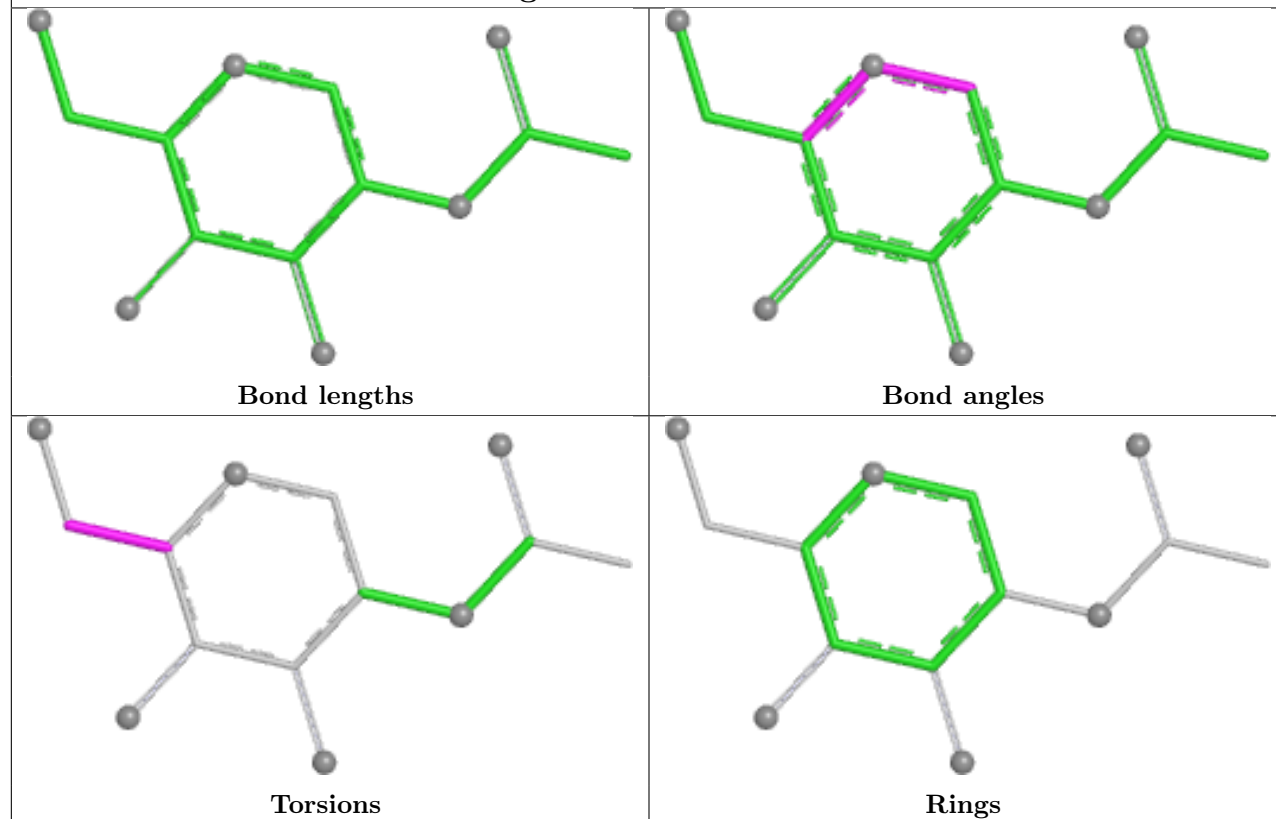


Ligand NAG B 2003

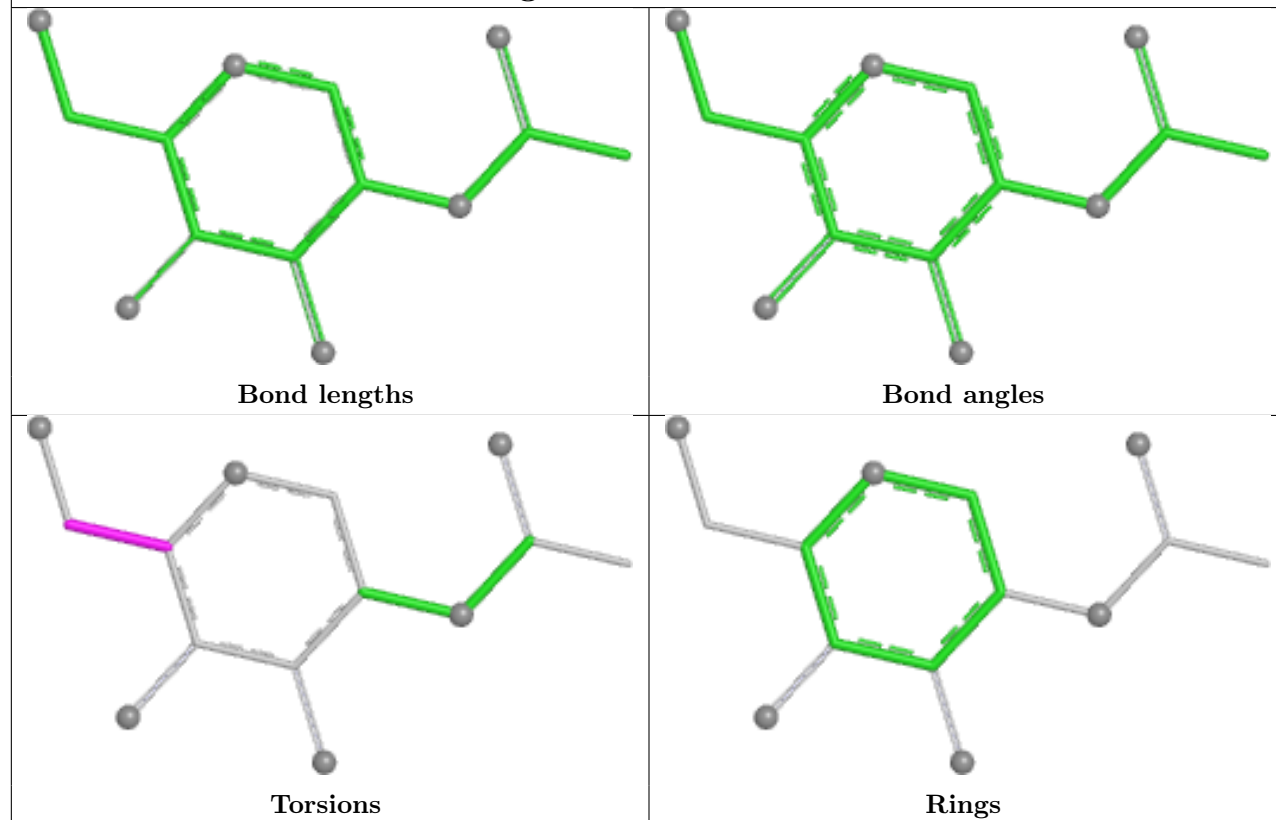


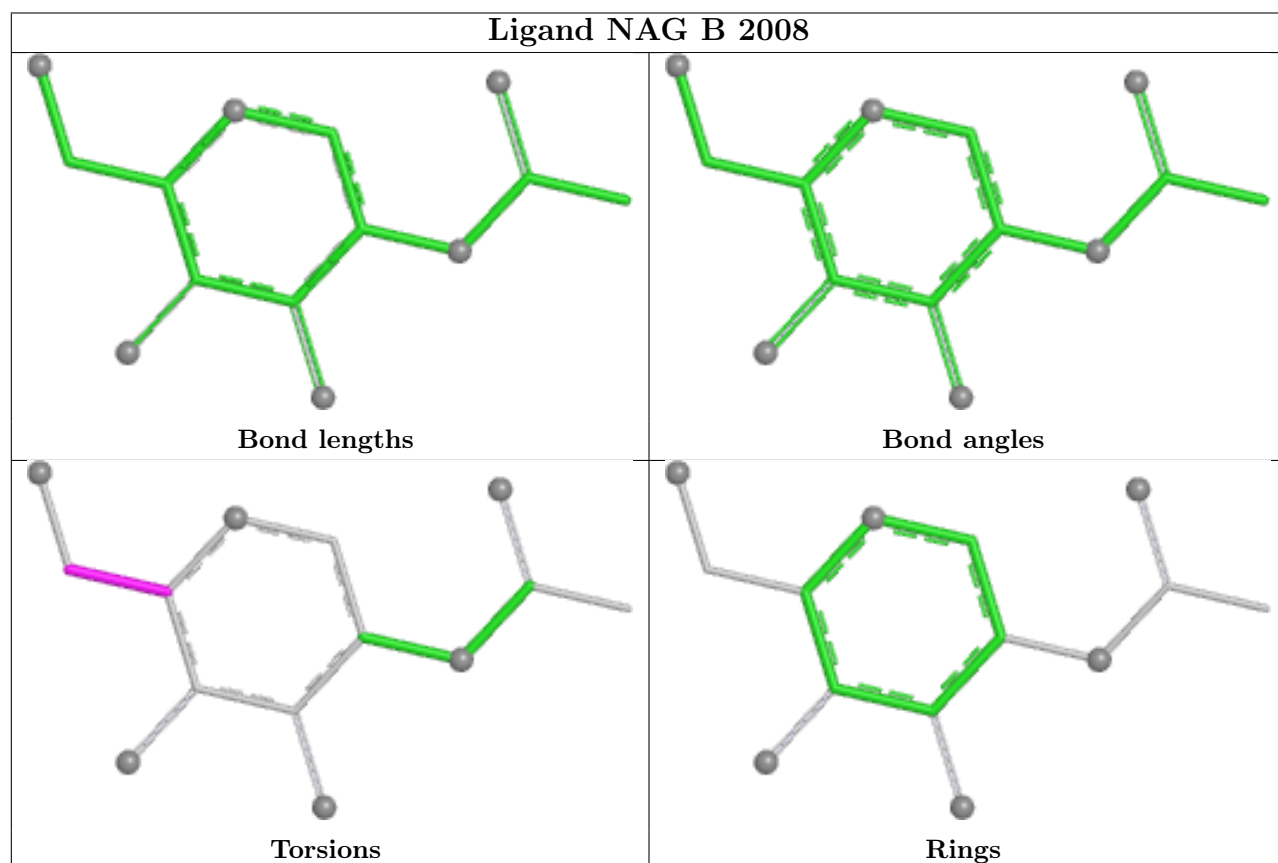
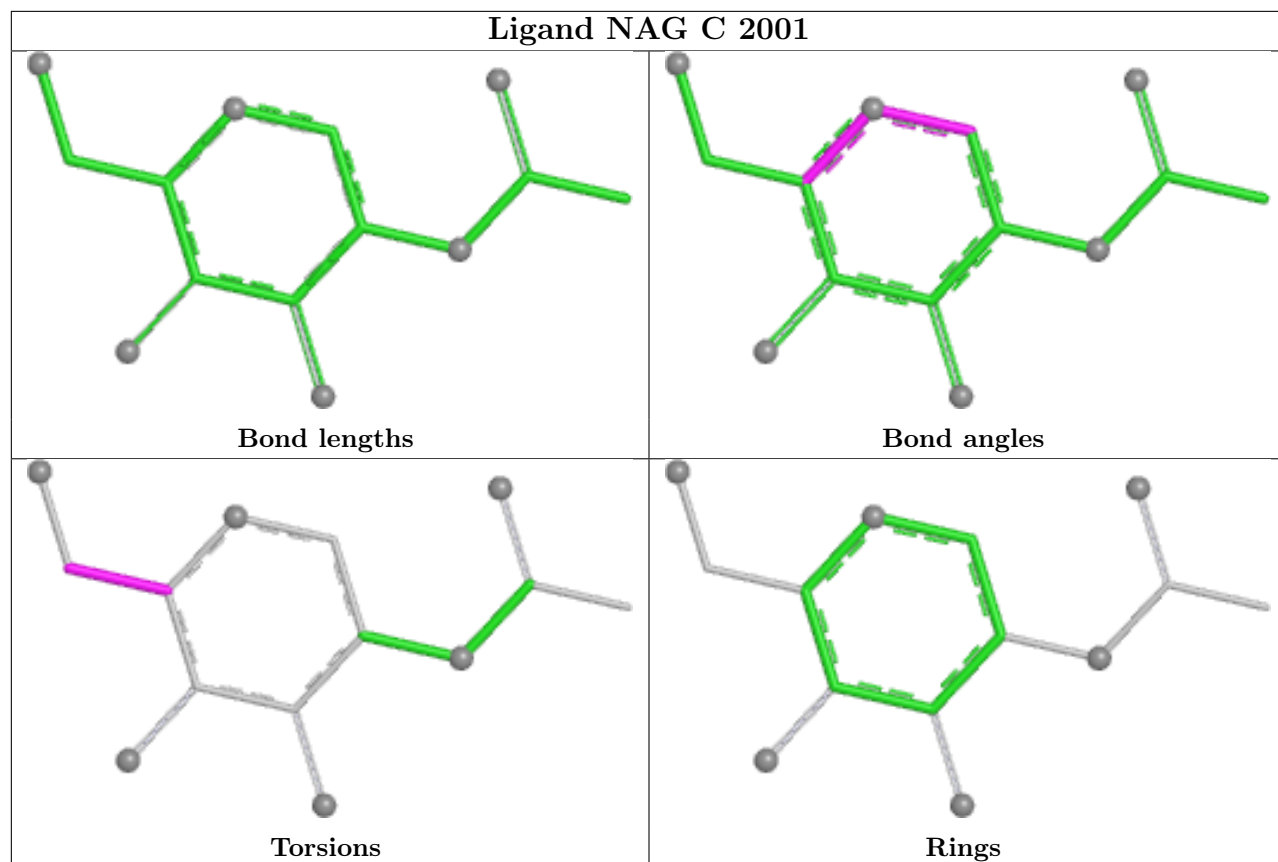


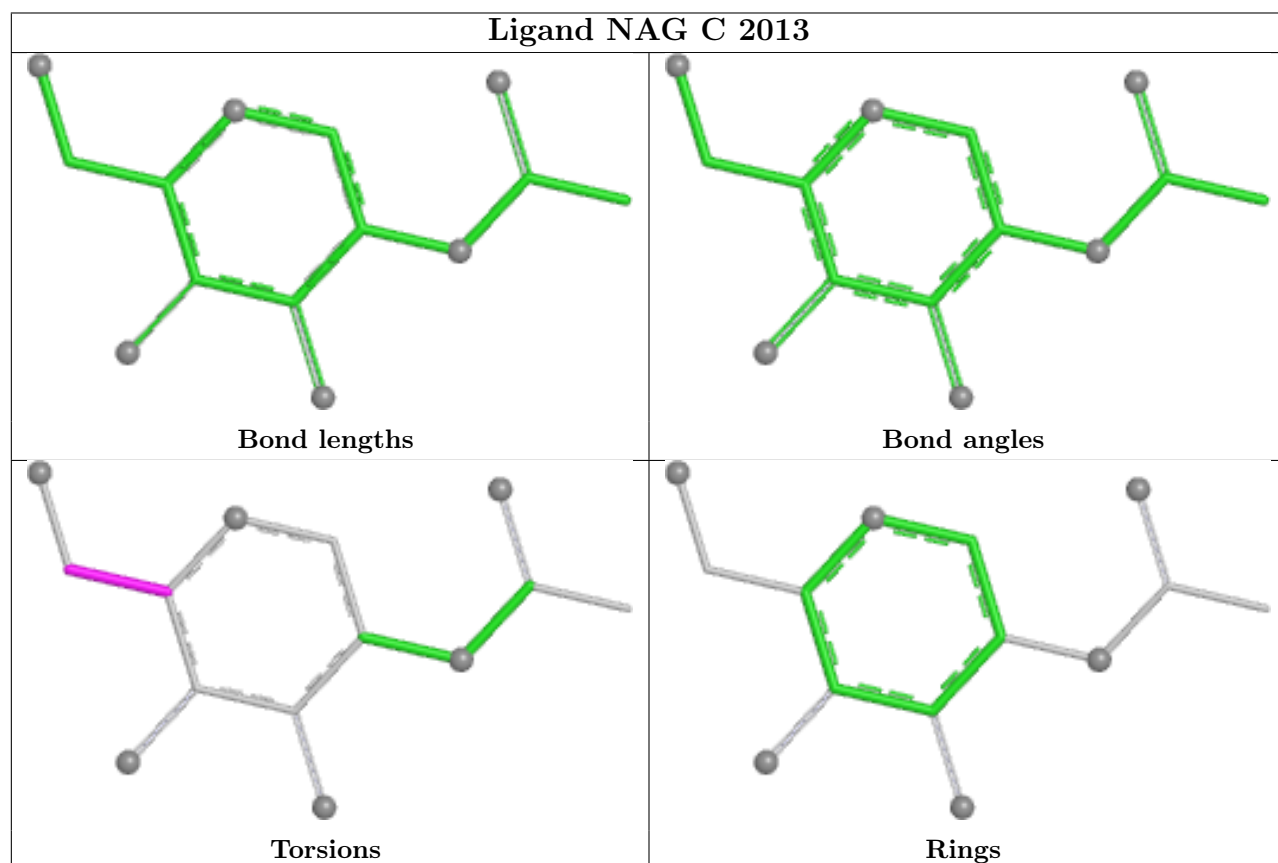
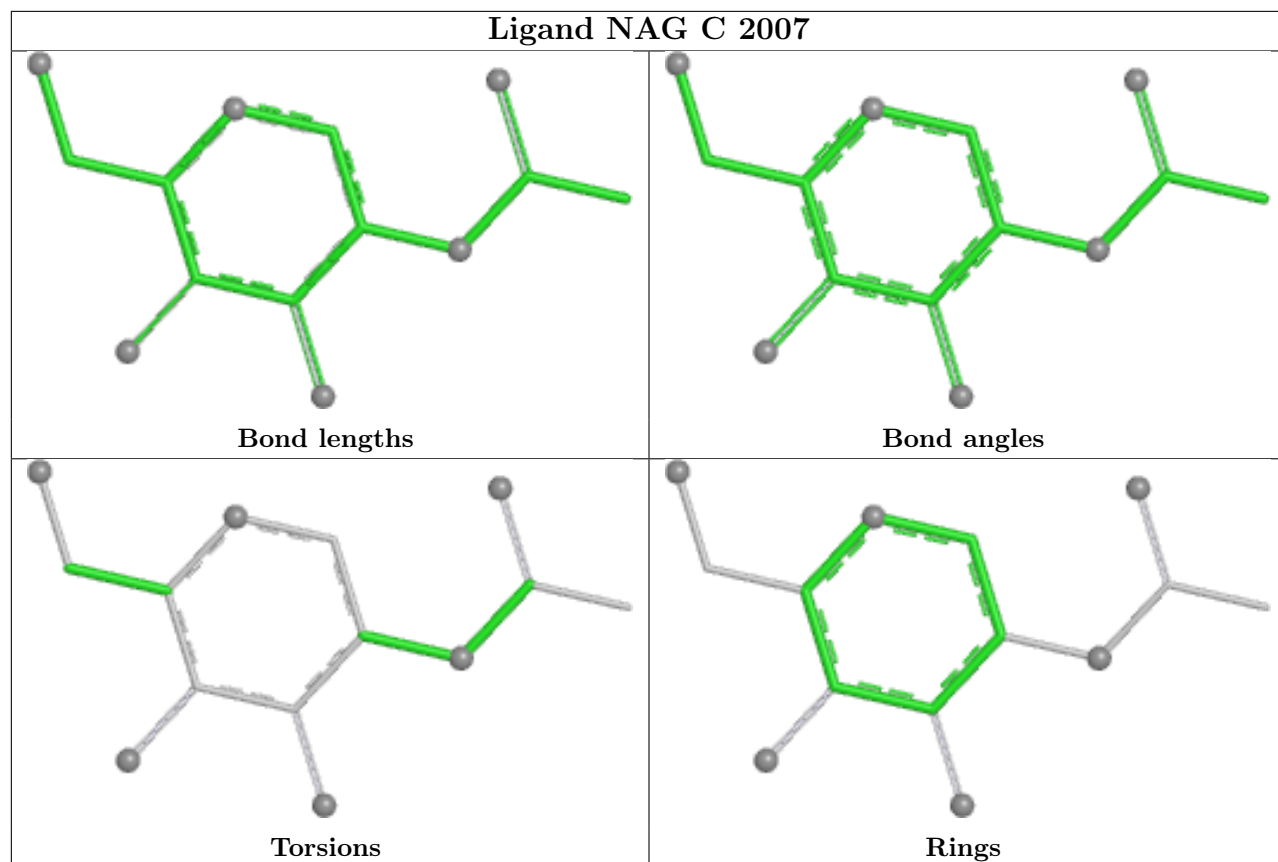
Ligand NAG B 2015



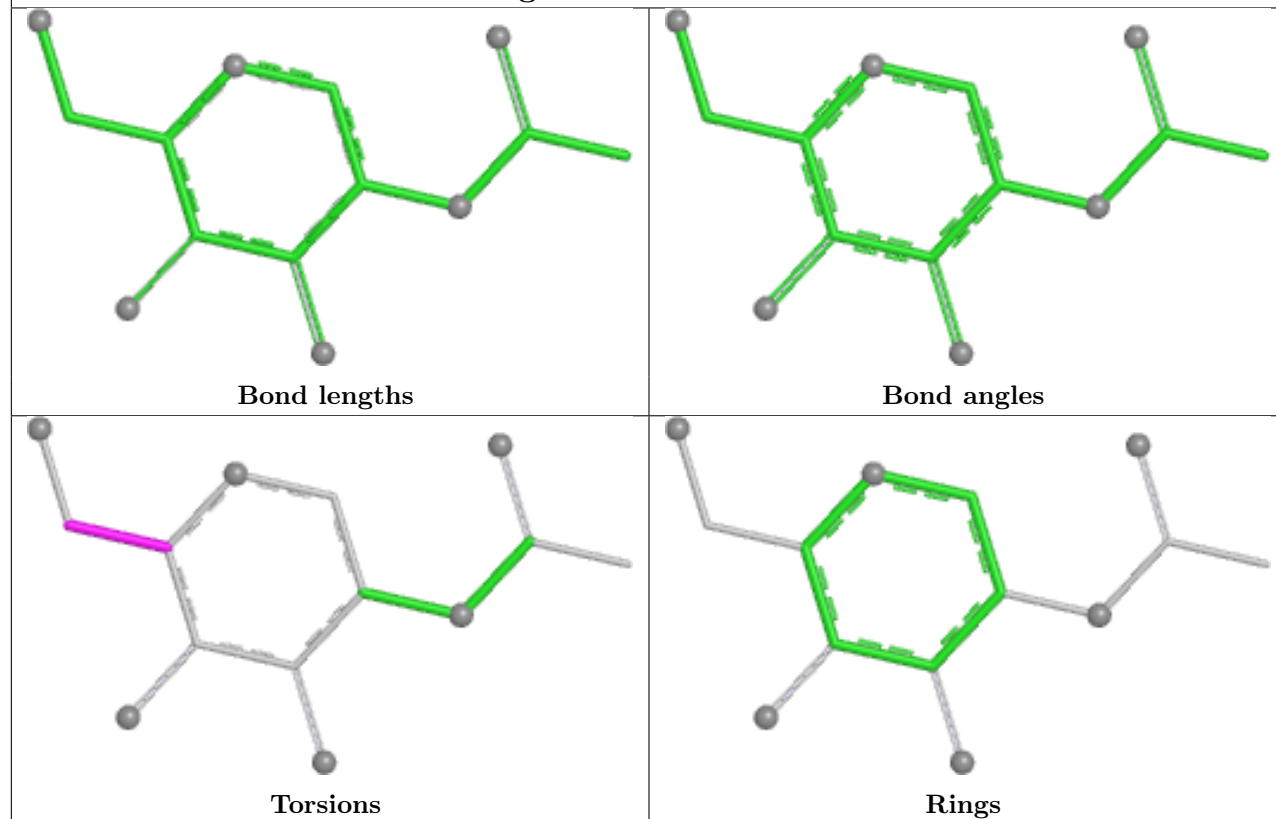
Ligand NAG C 2002



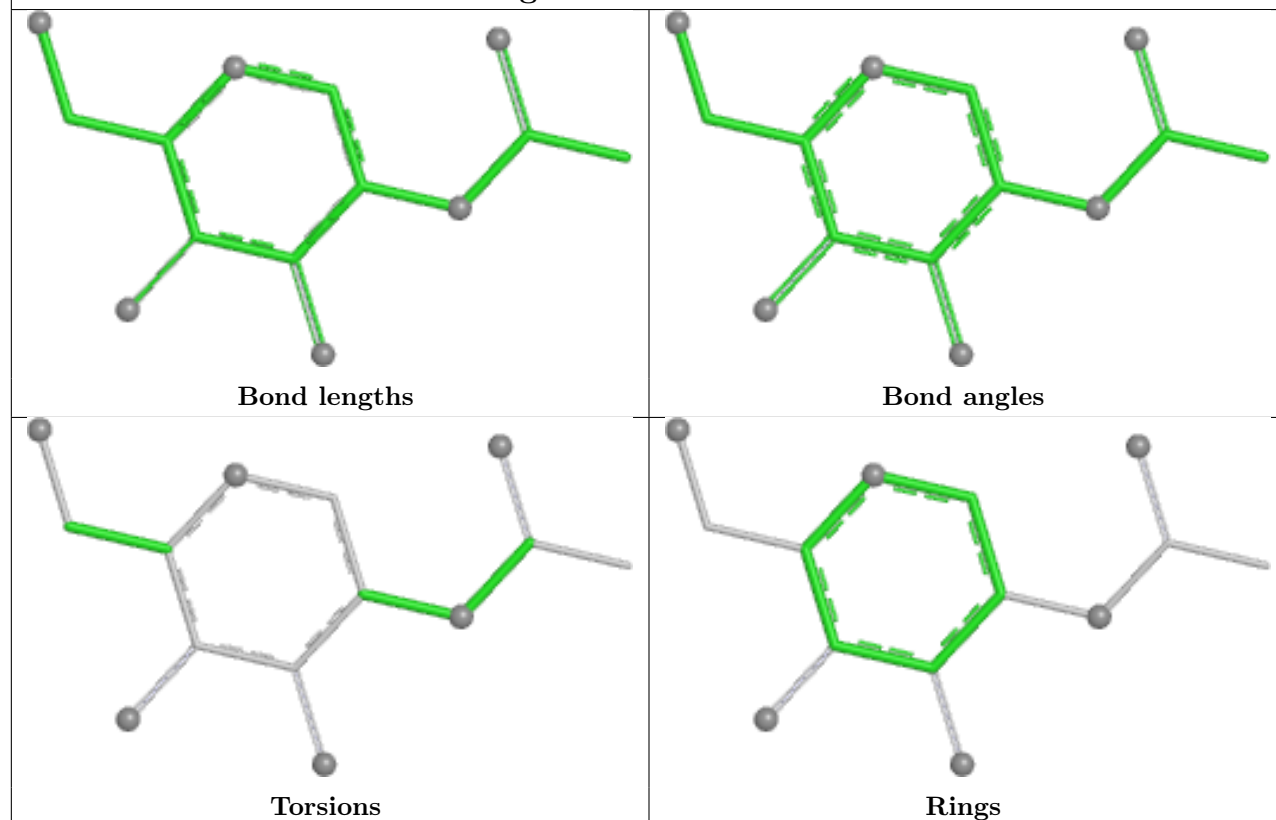


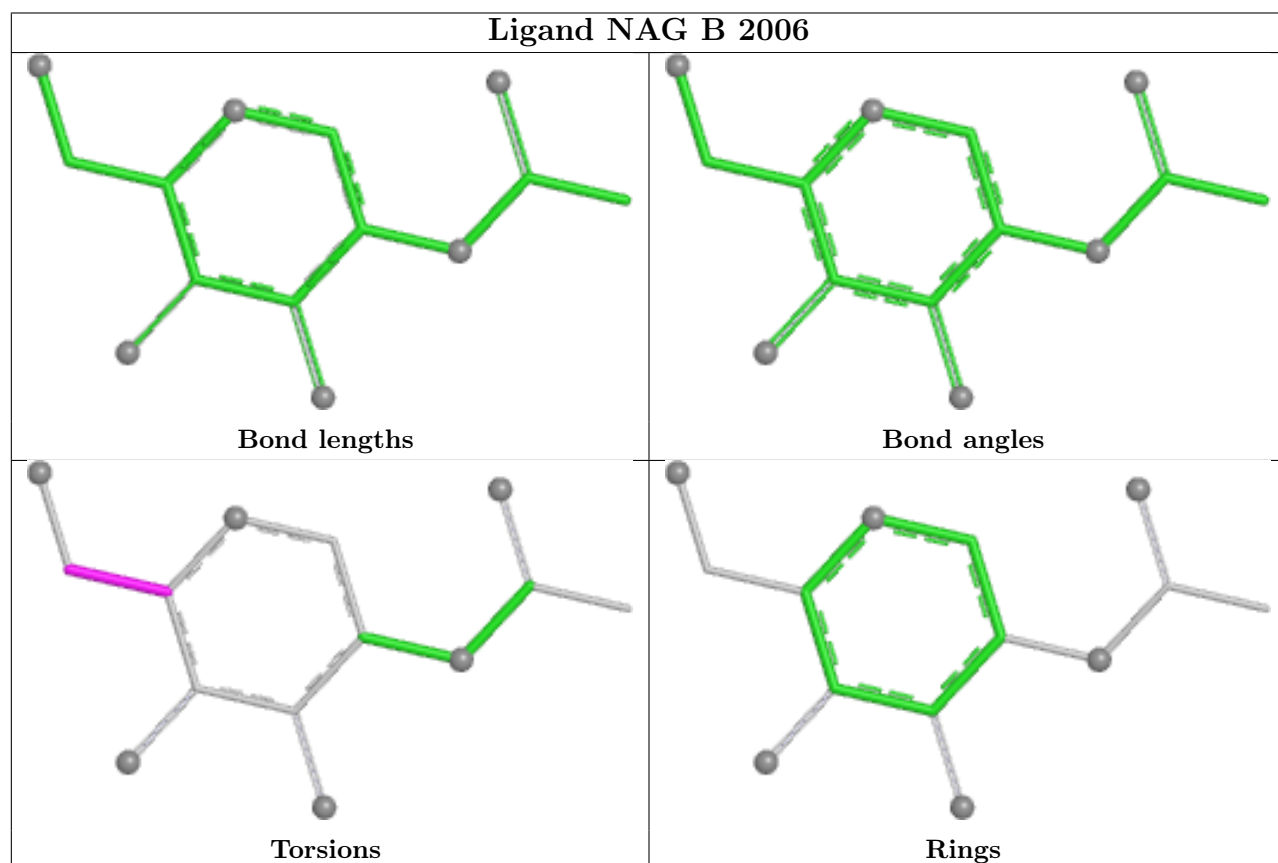
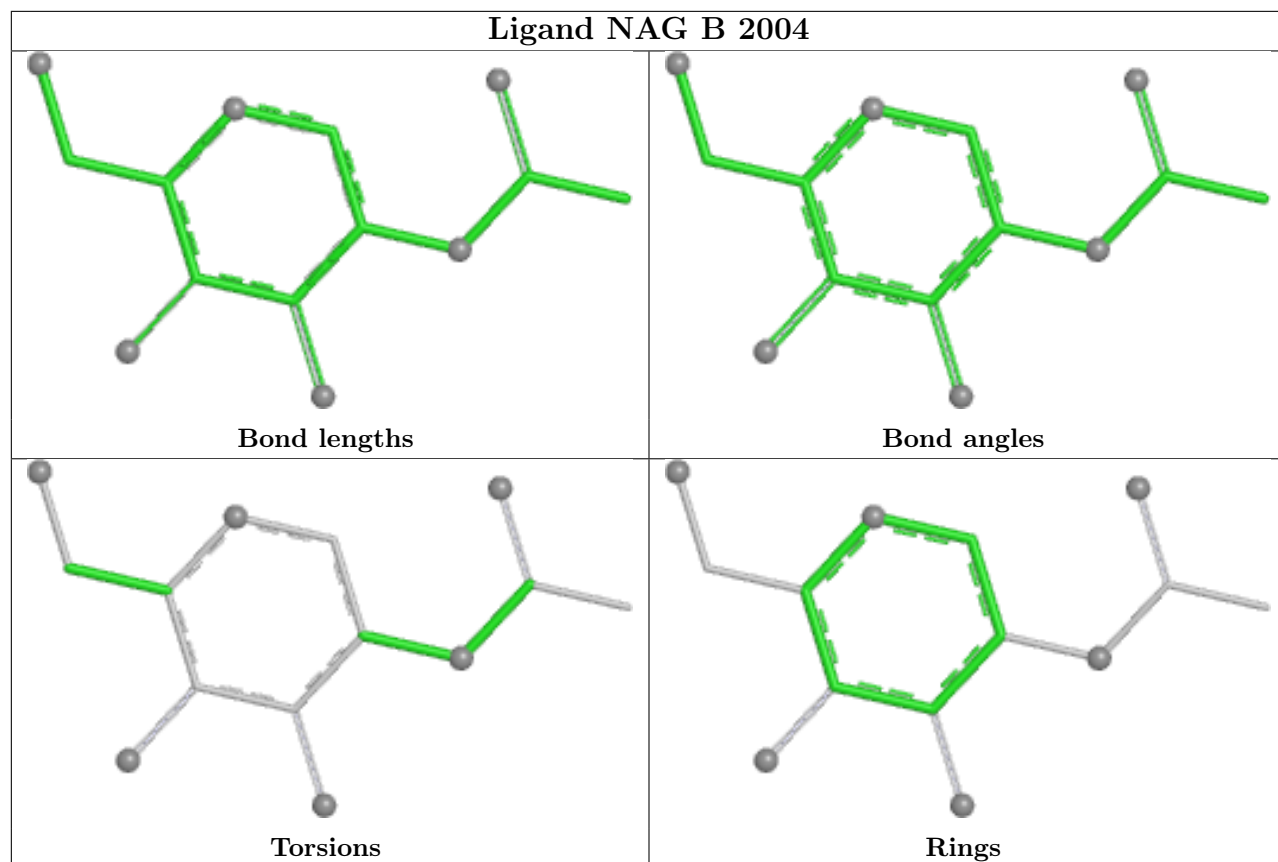


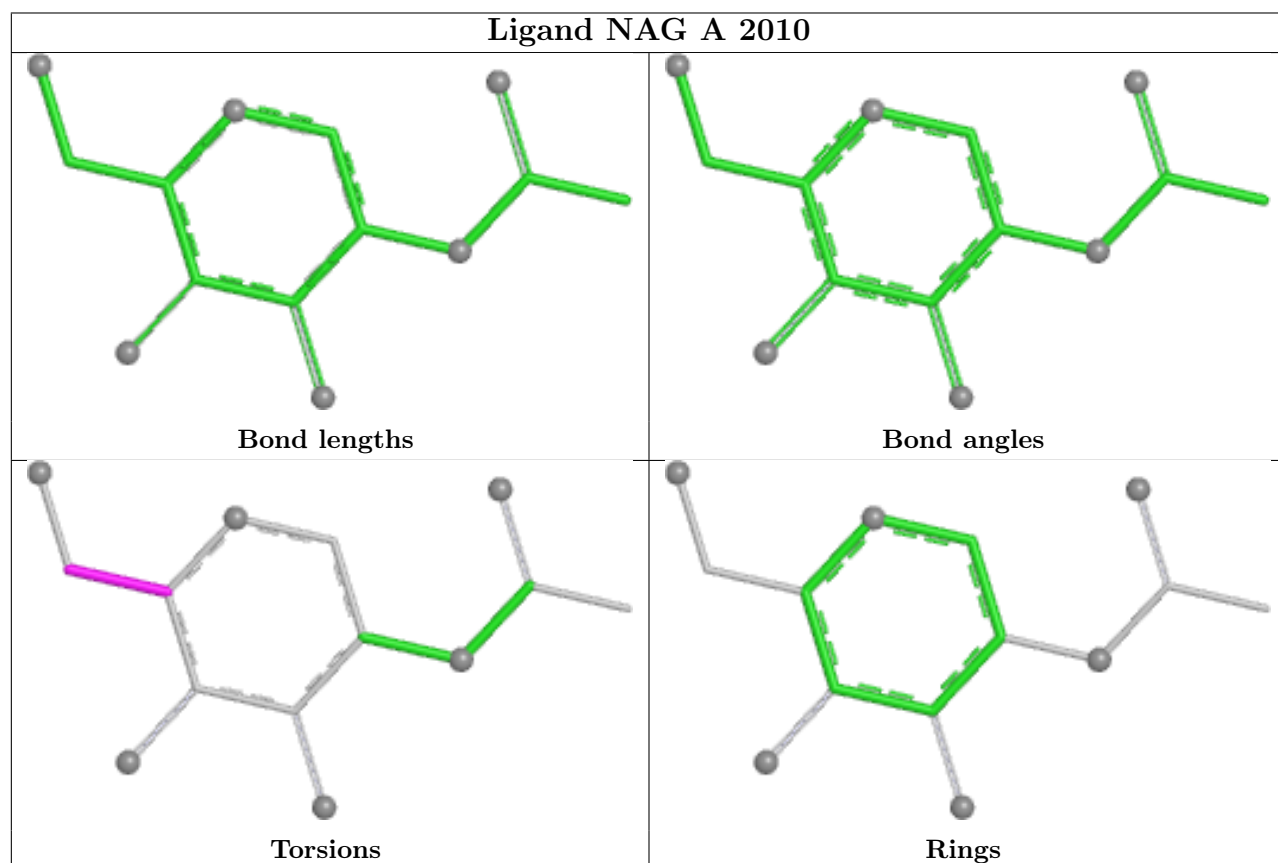
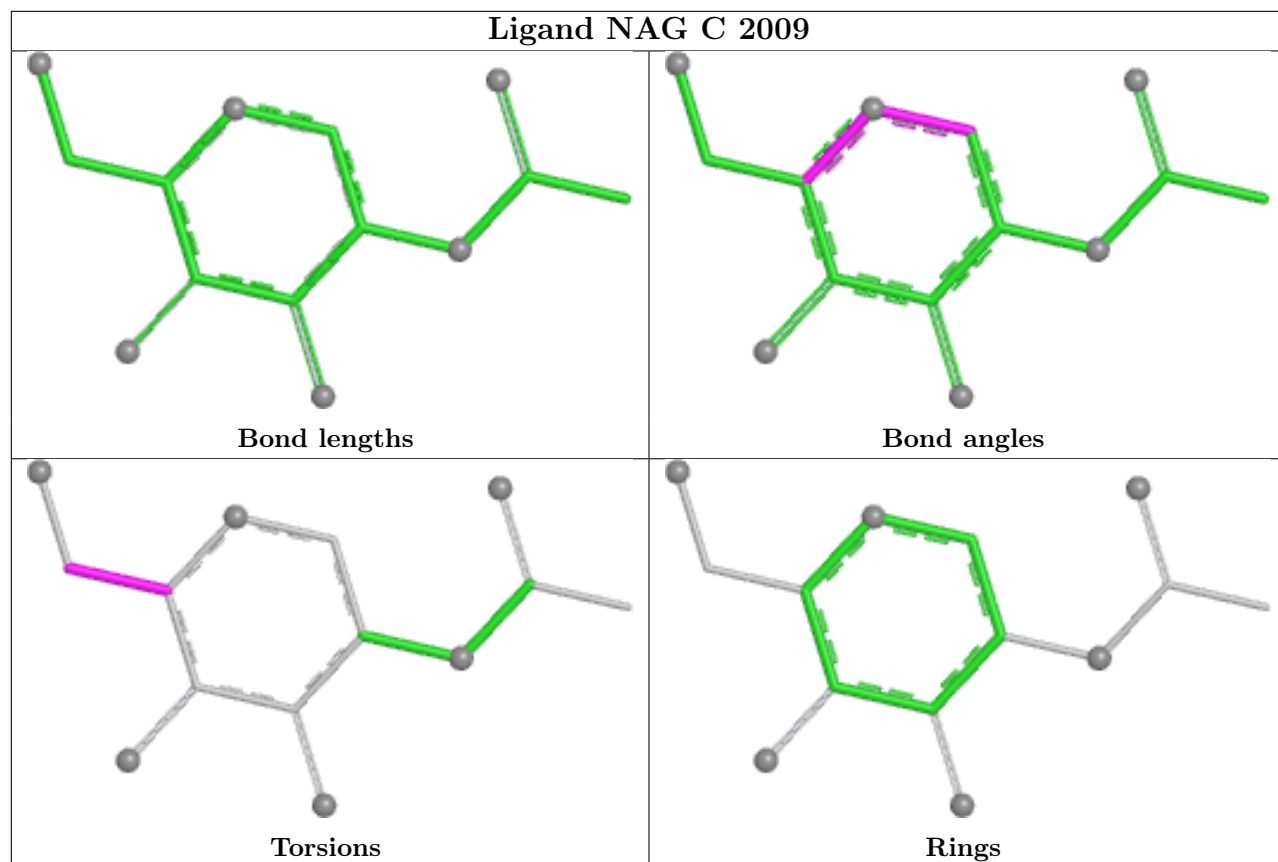
Ligand NAG A 2007

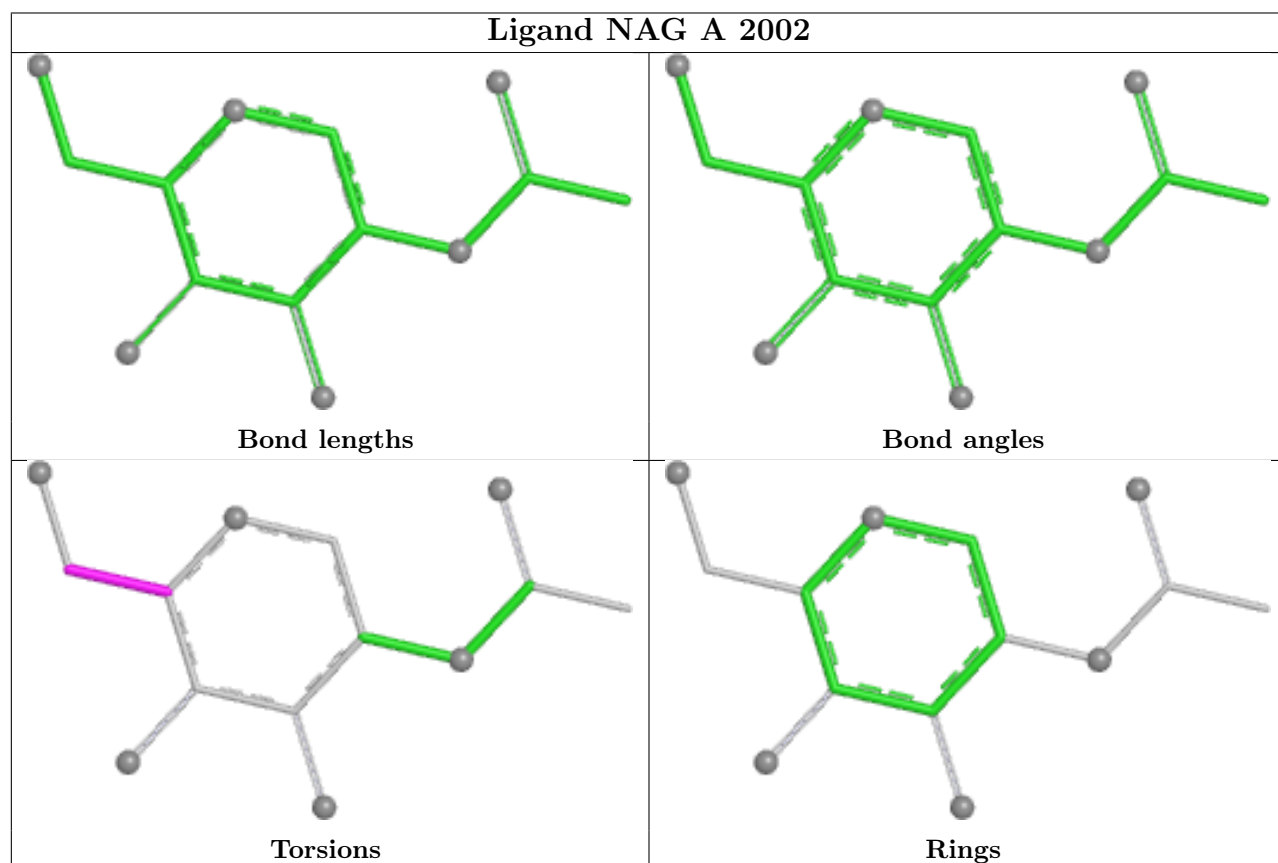
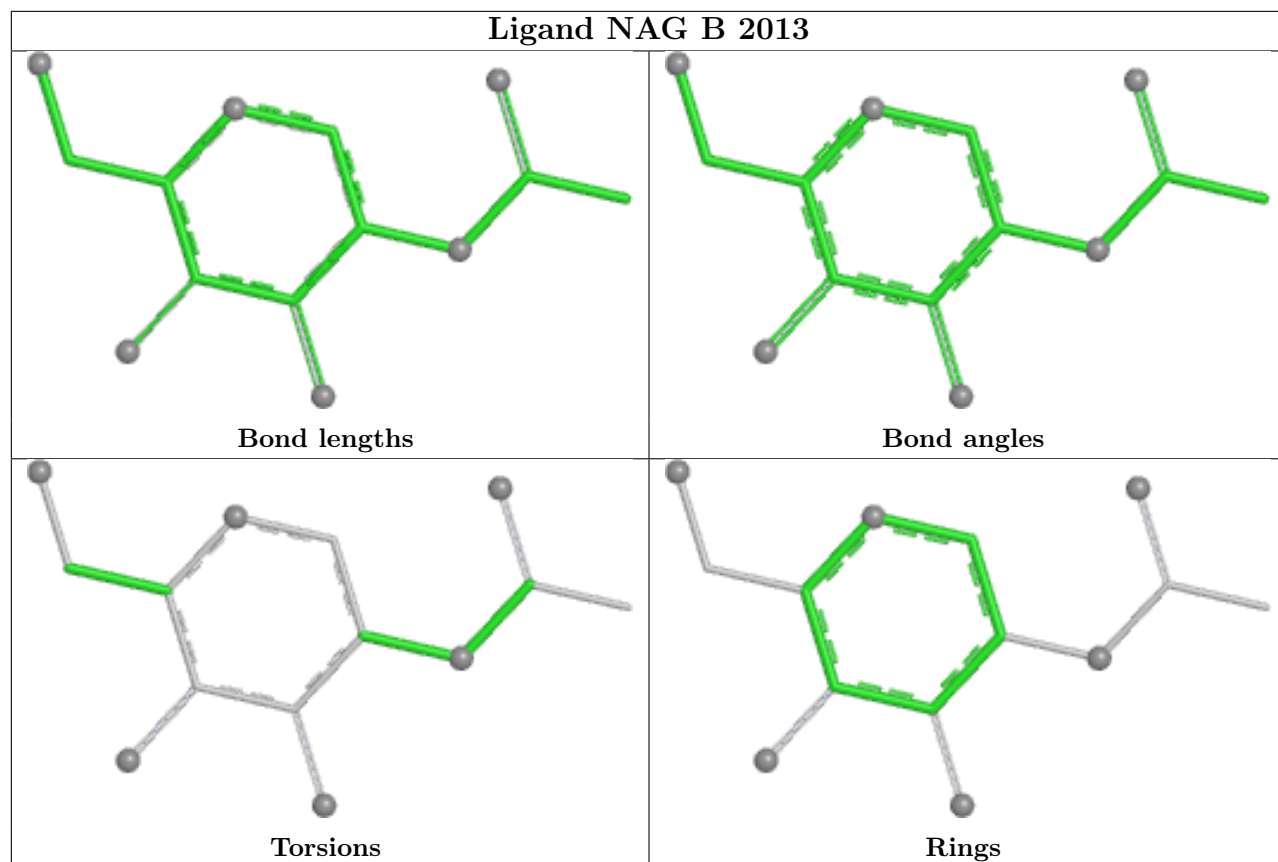


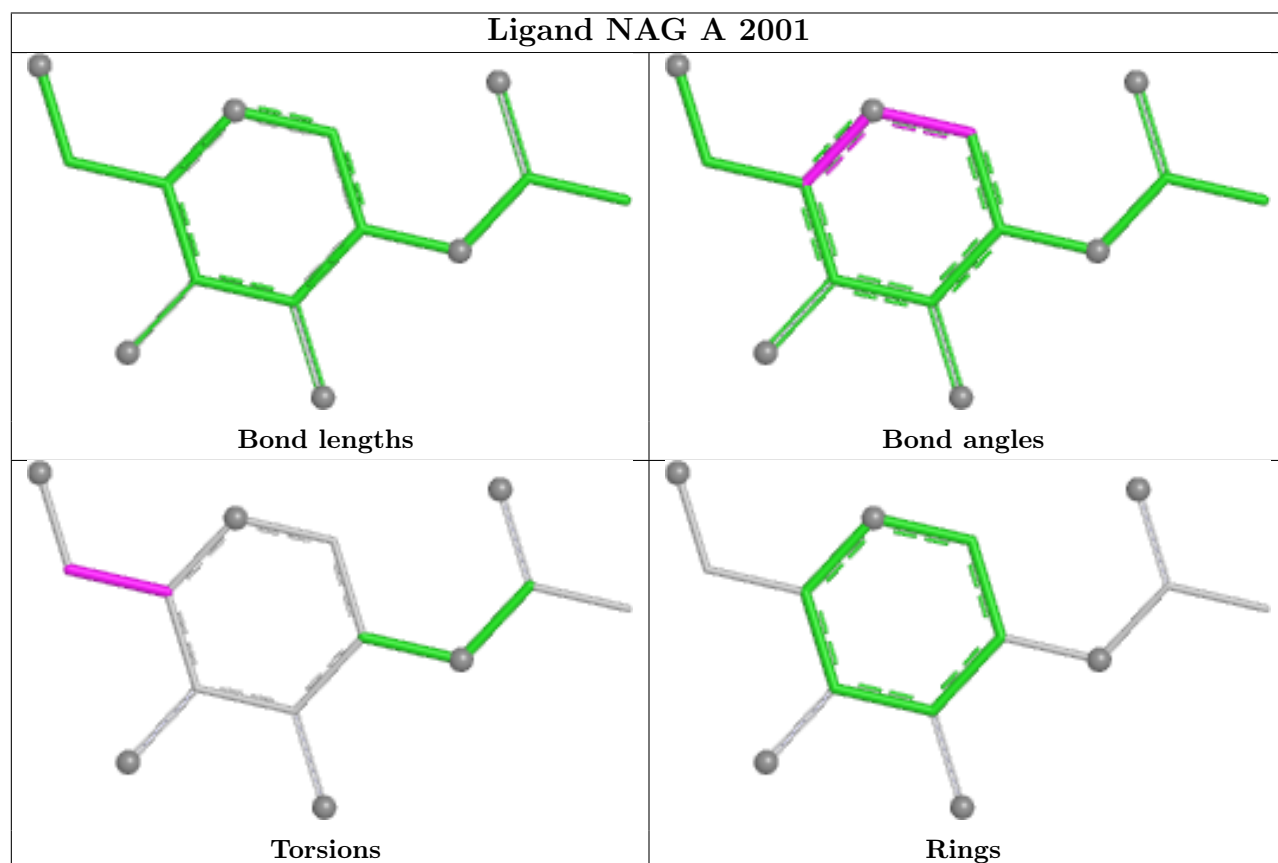
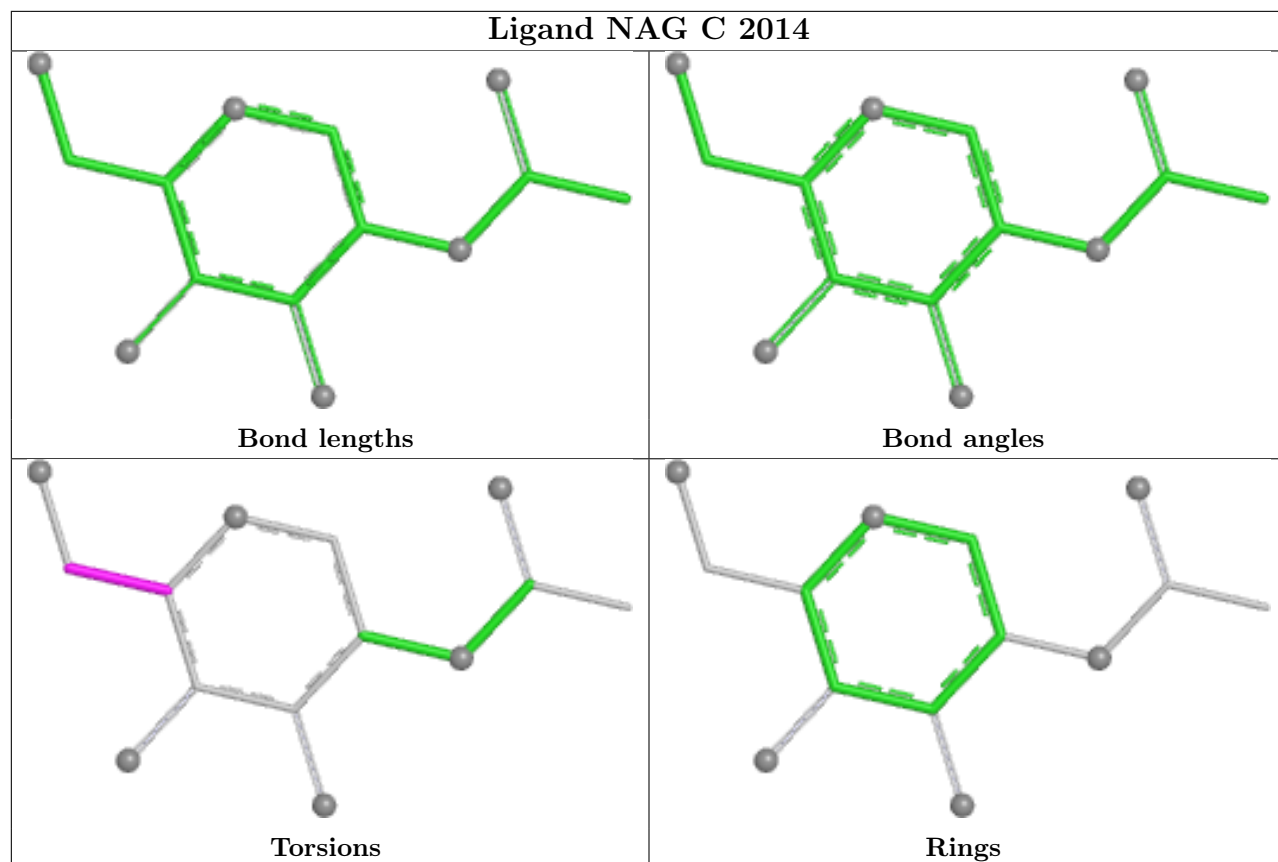
Ligand NAG B 2009



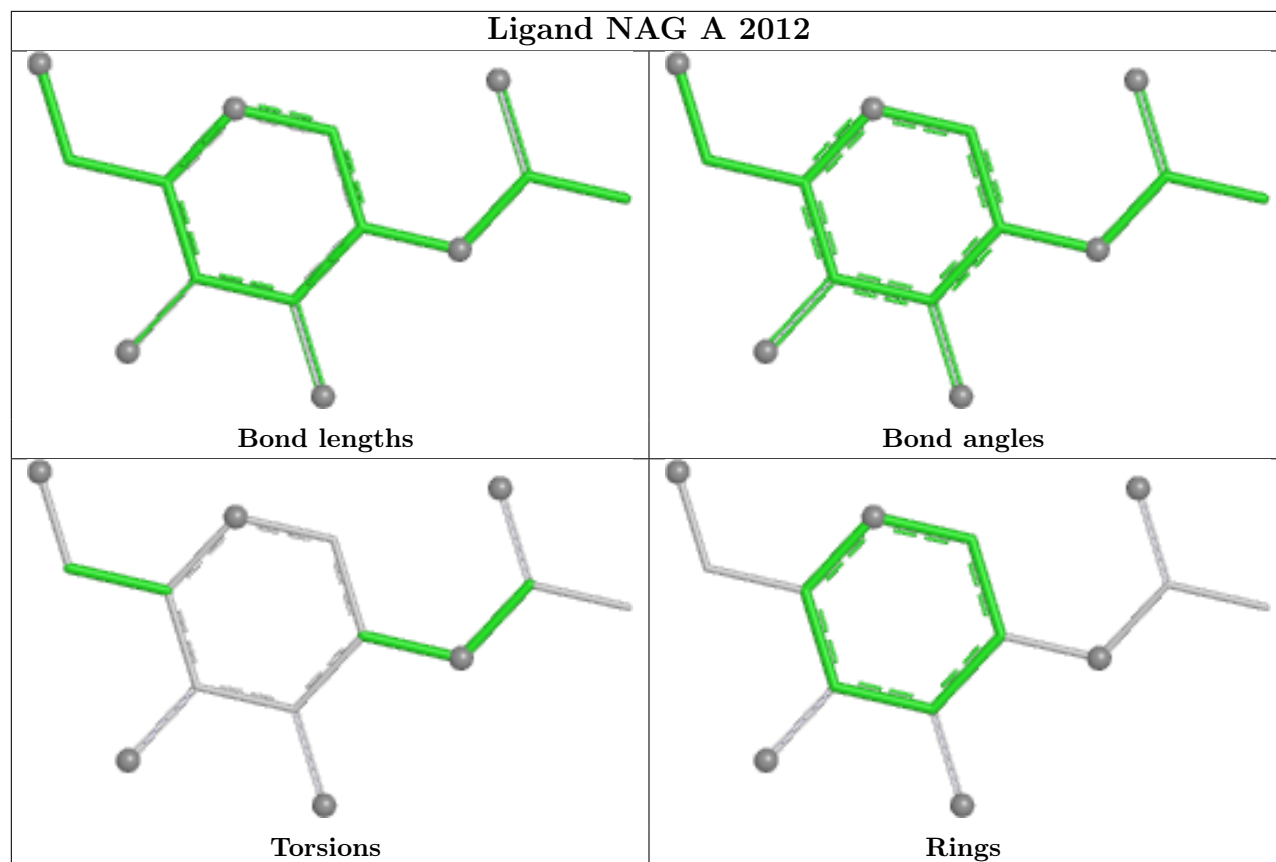




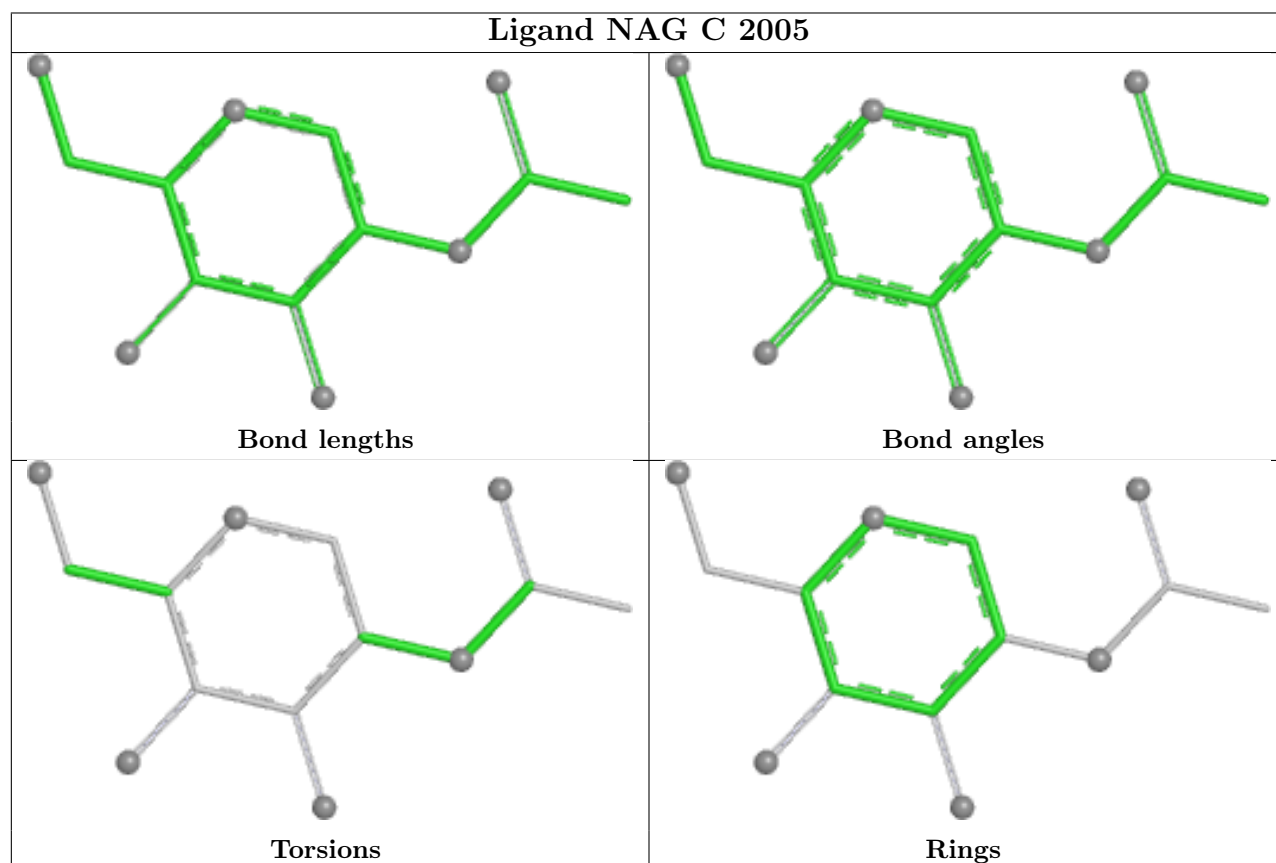




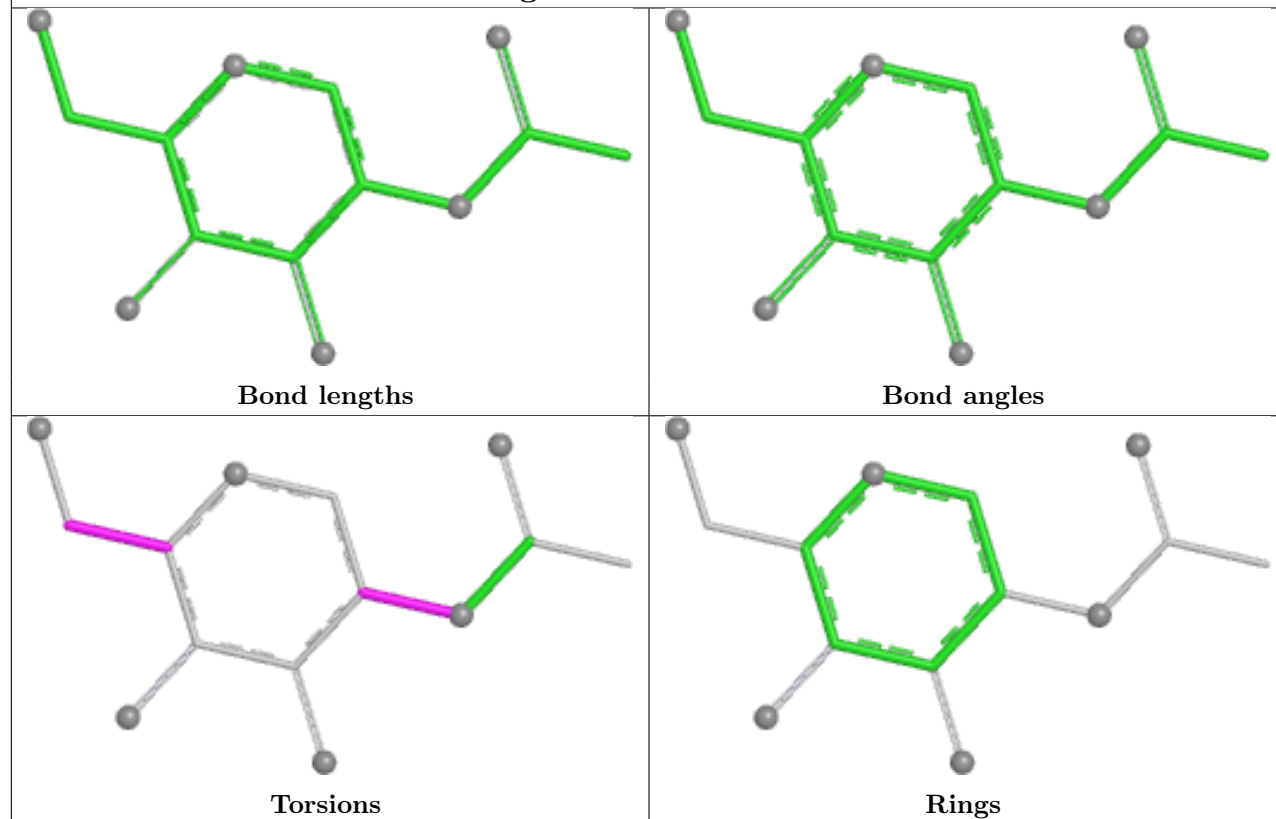
Ligand NAG A 2012



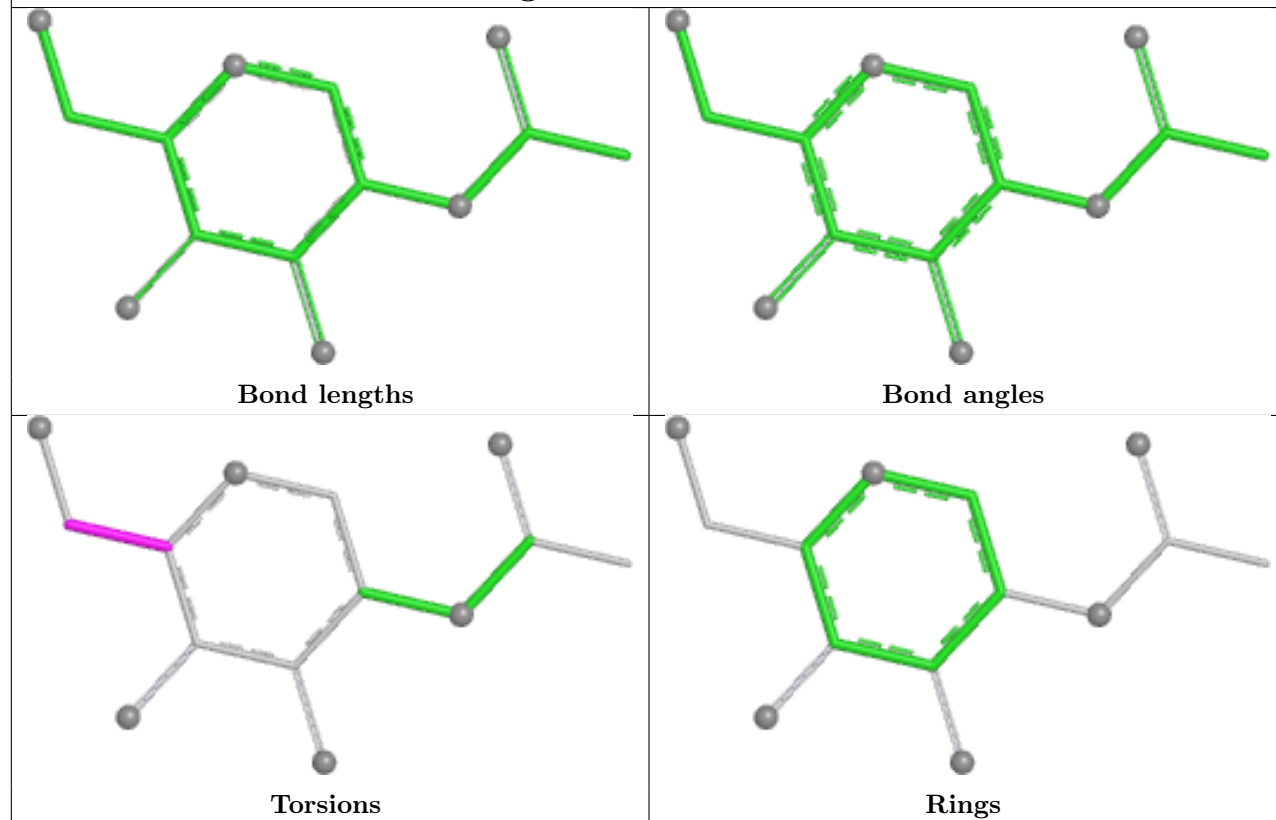
Ligand NAG C 2005

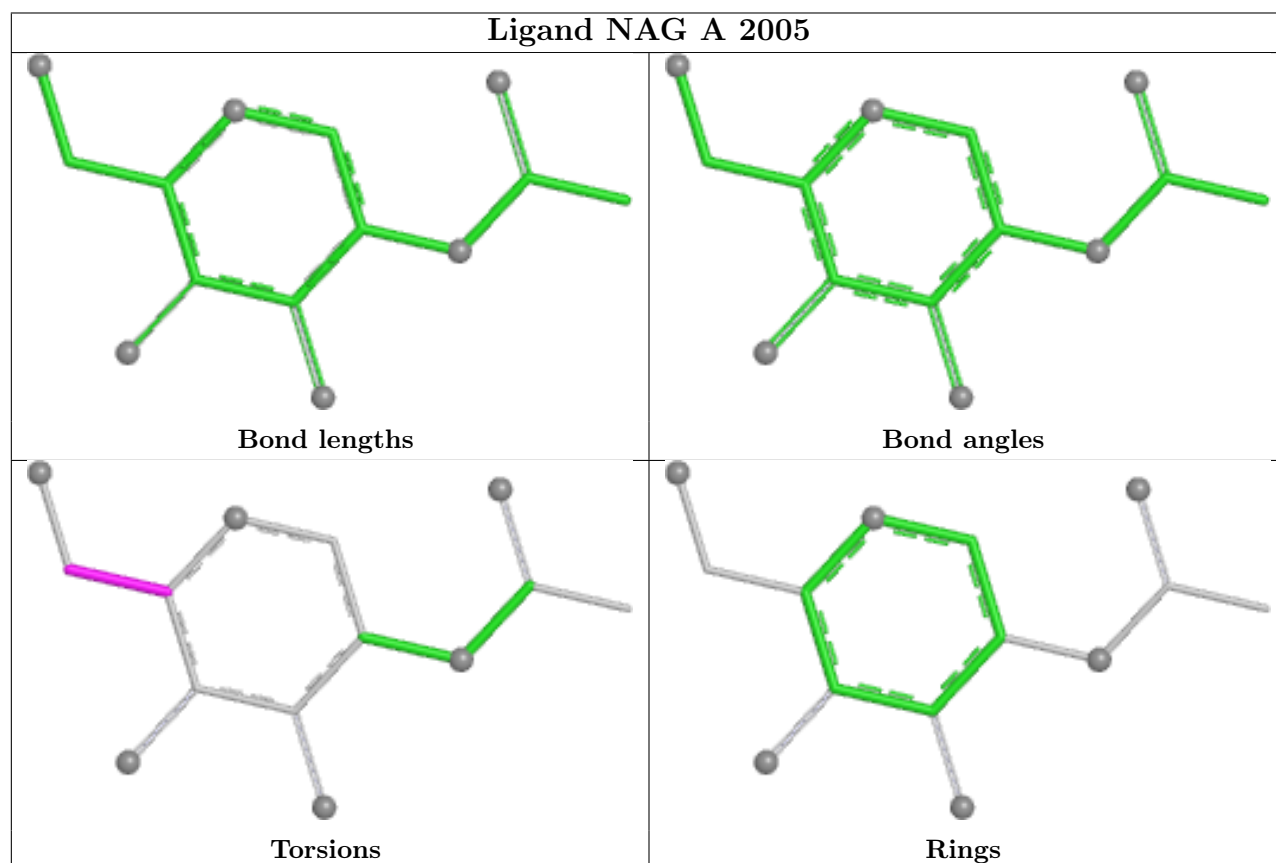
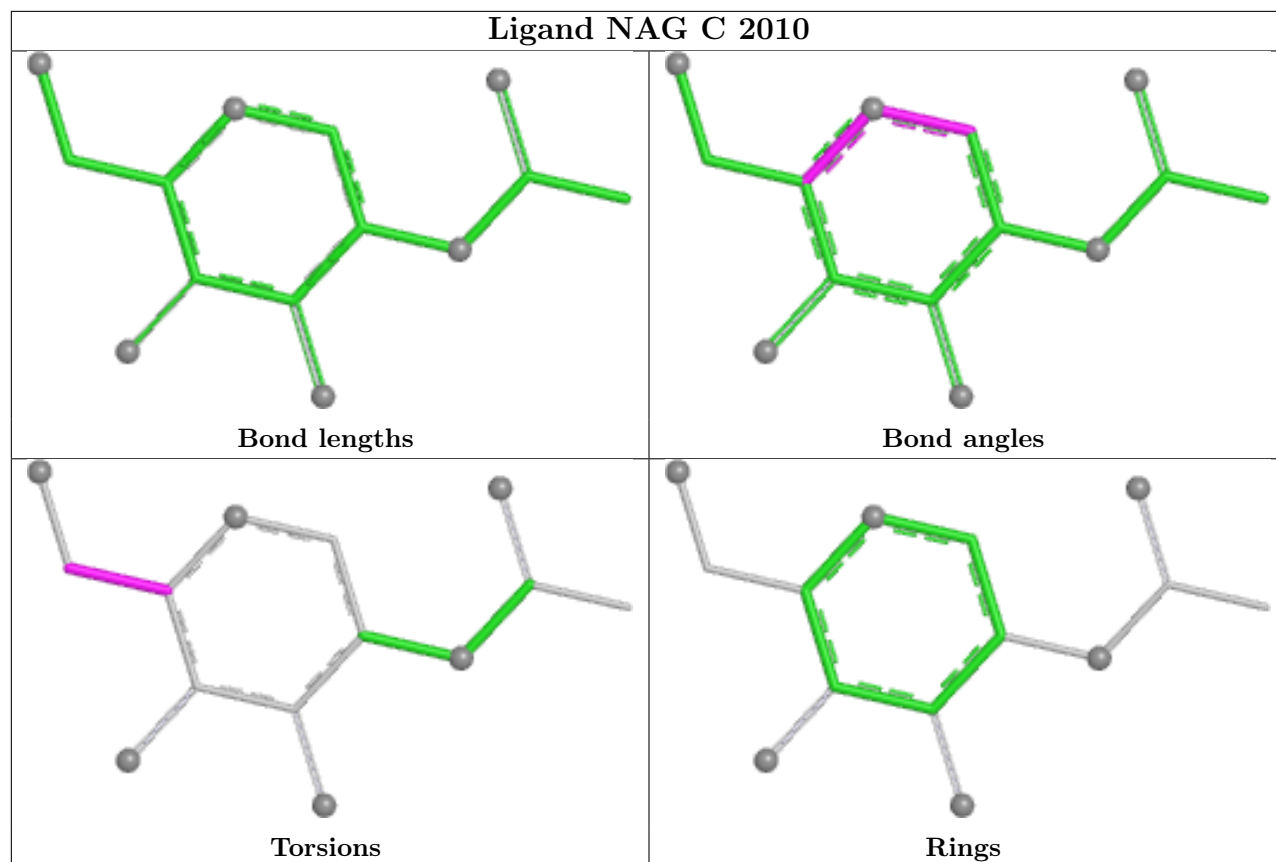


Ligand NAG B 2002

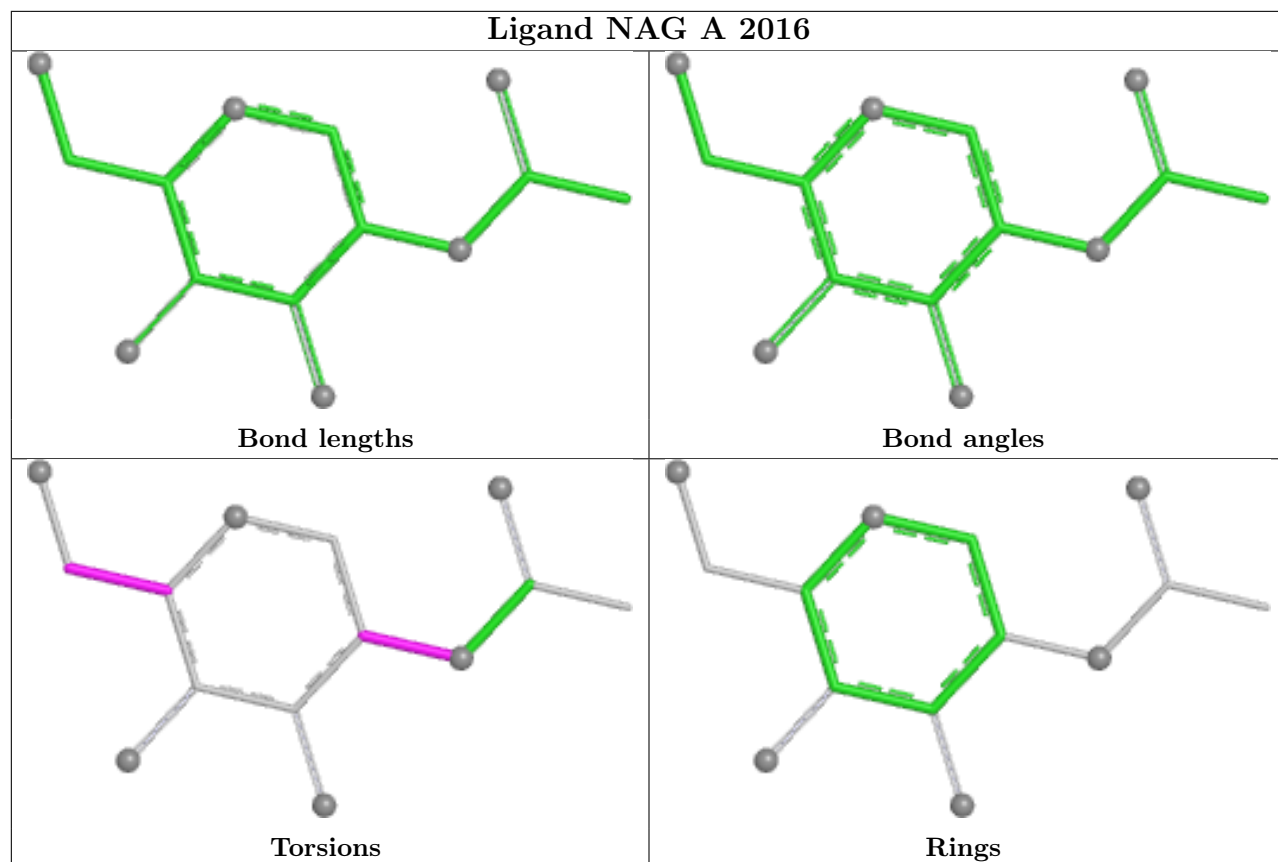


Ligand NAG C 2003

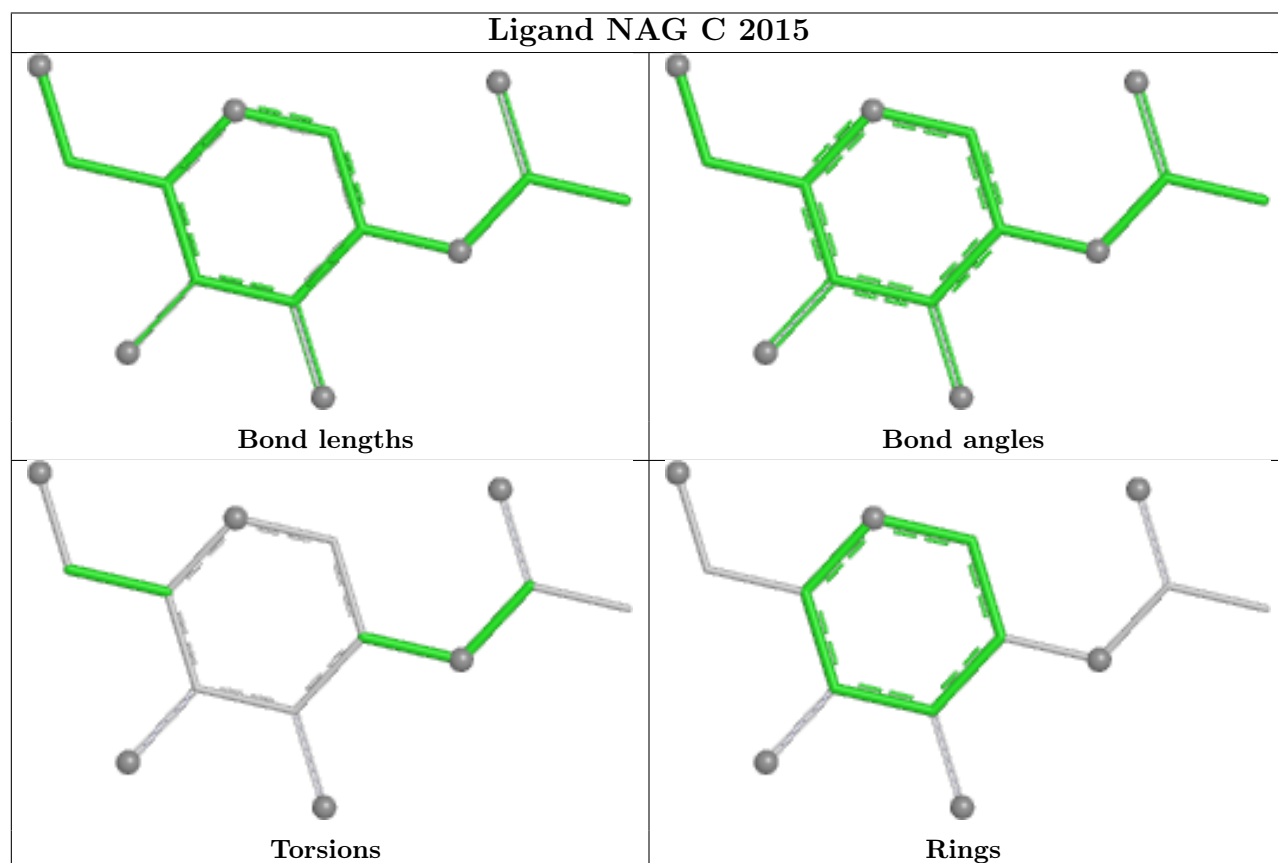


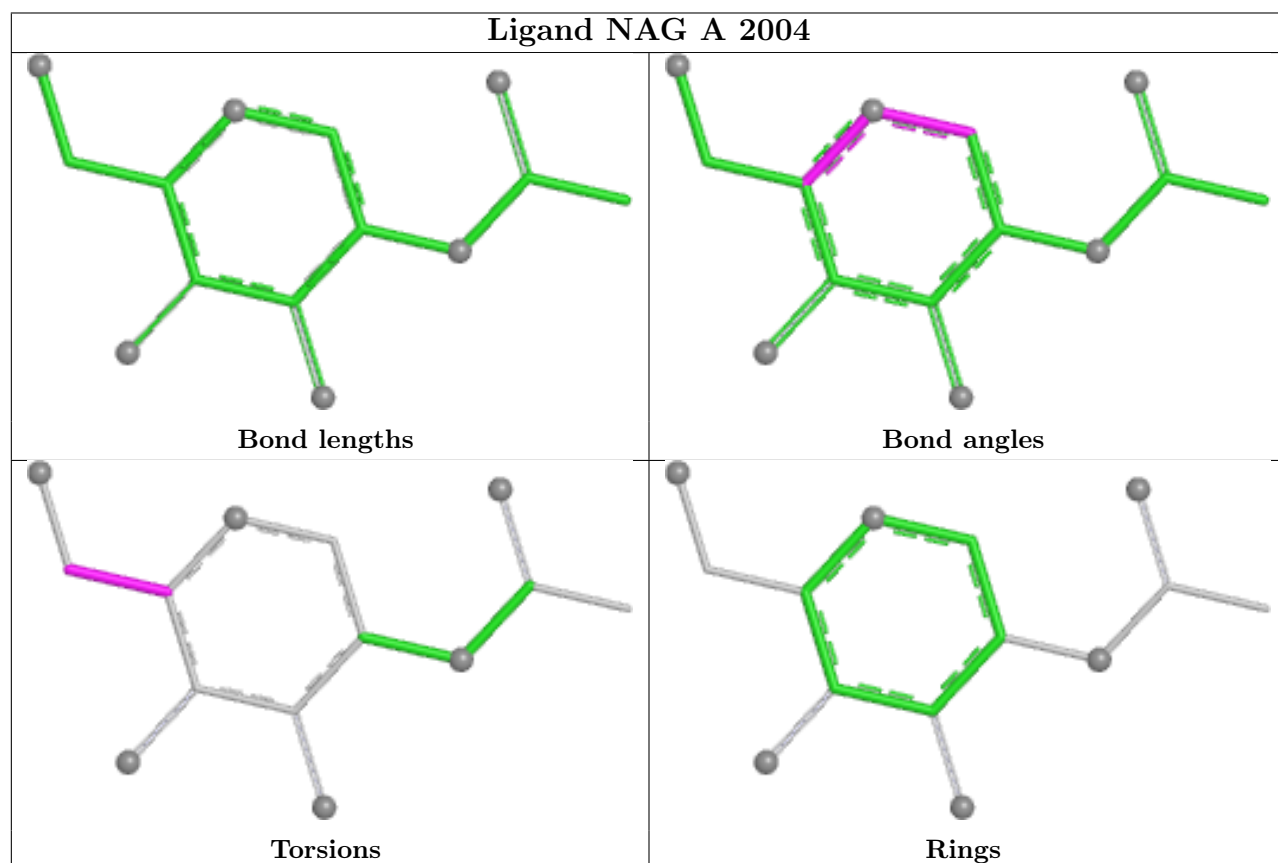
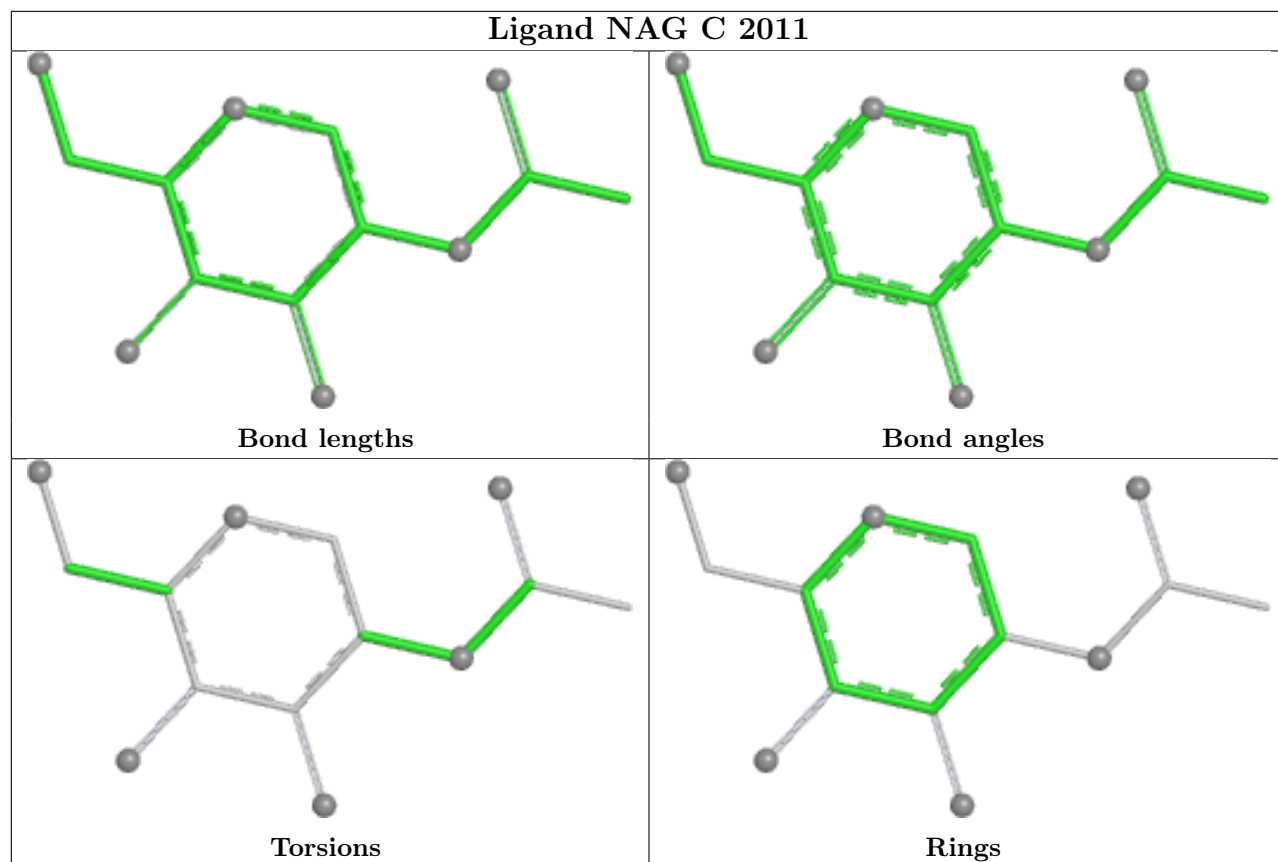


Ligand NAG A 2016

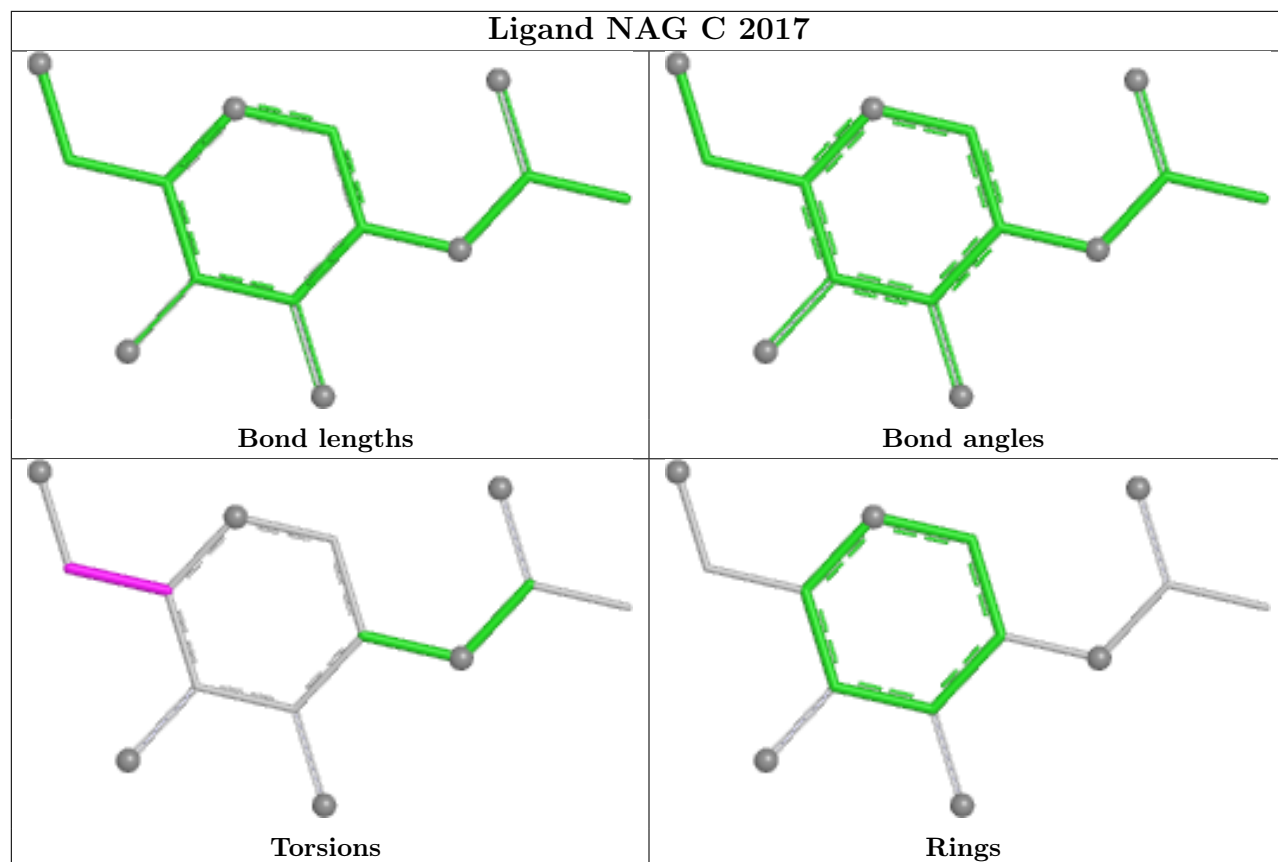


Ligand NAG C 2015

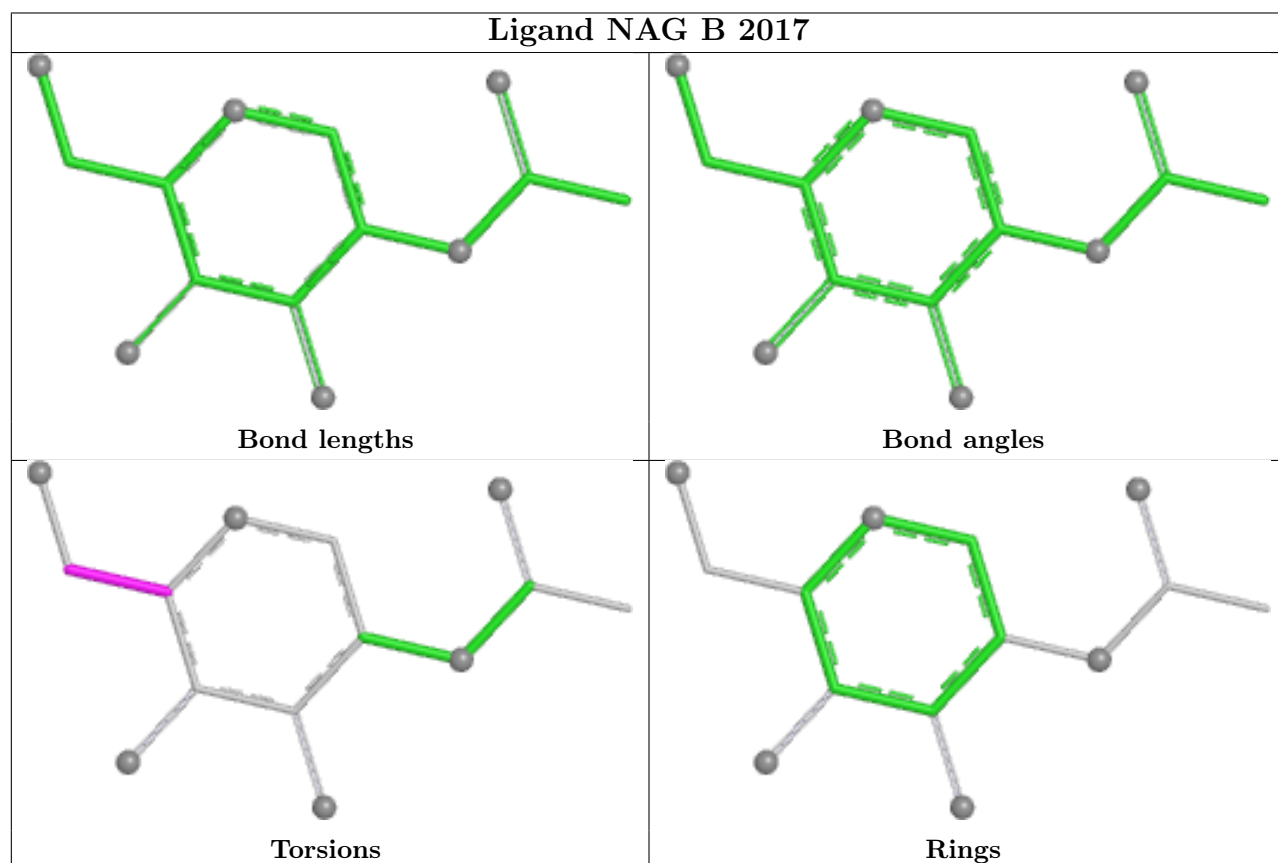


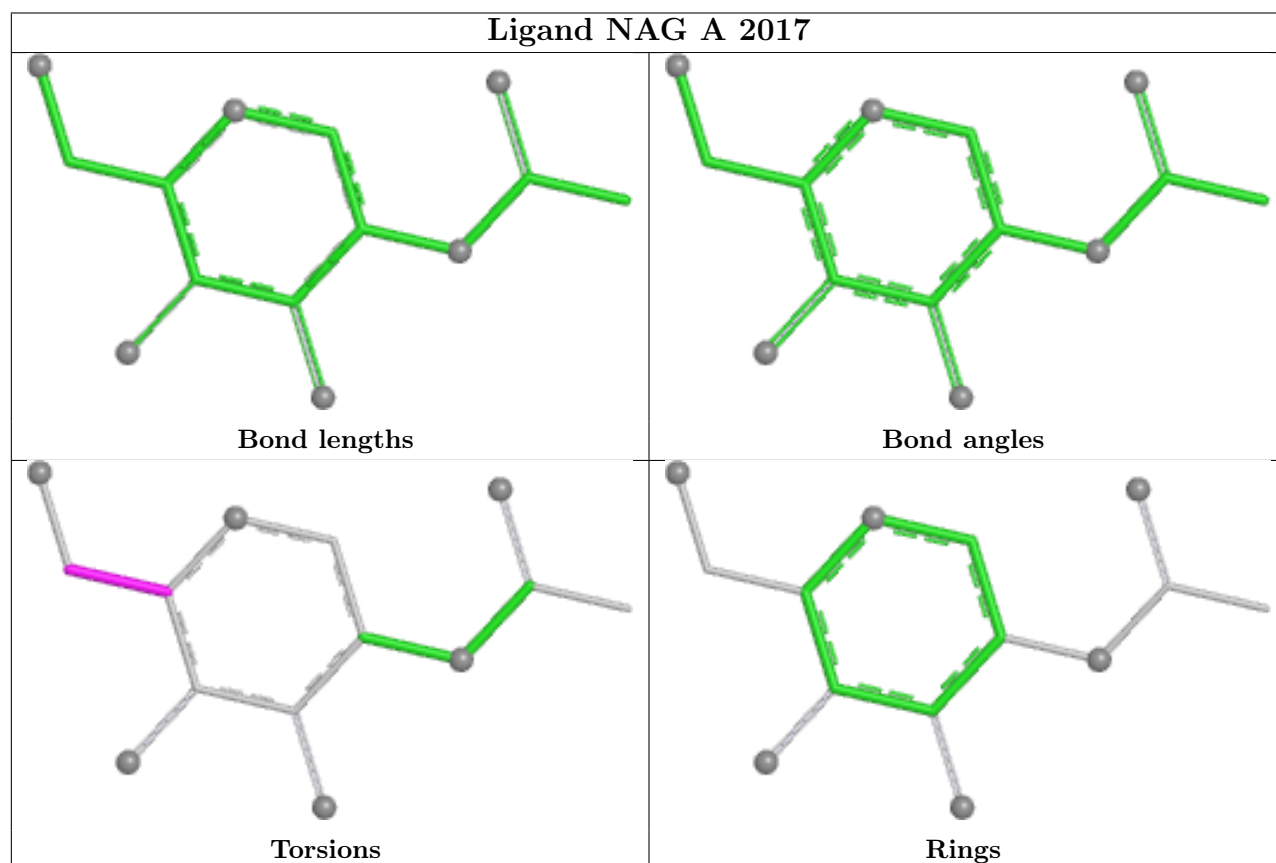
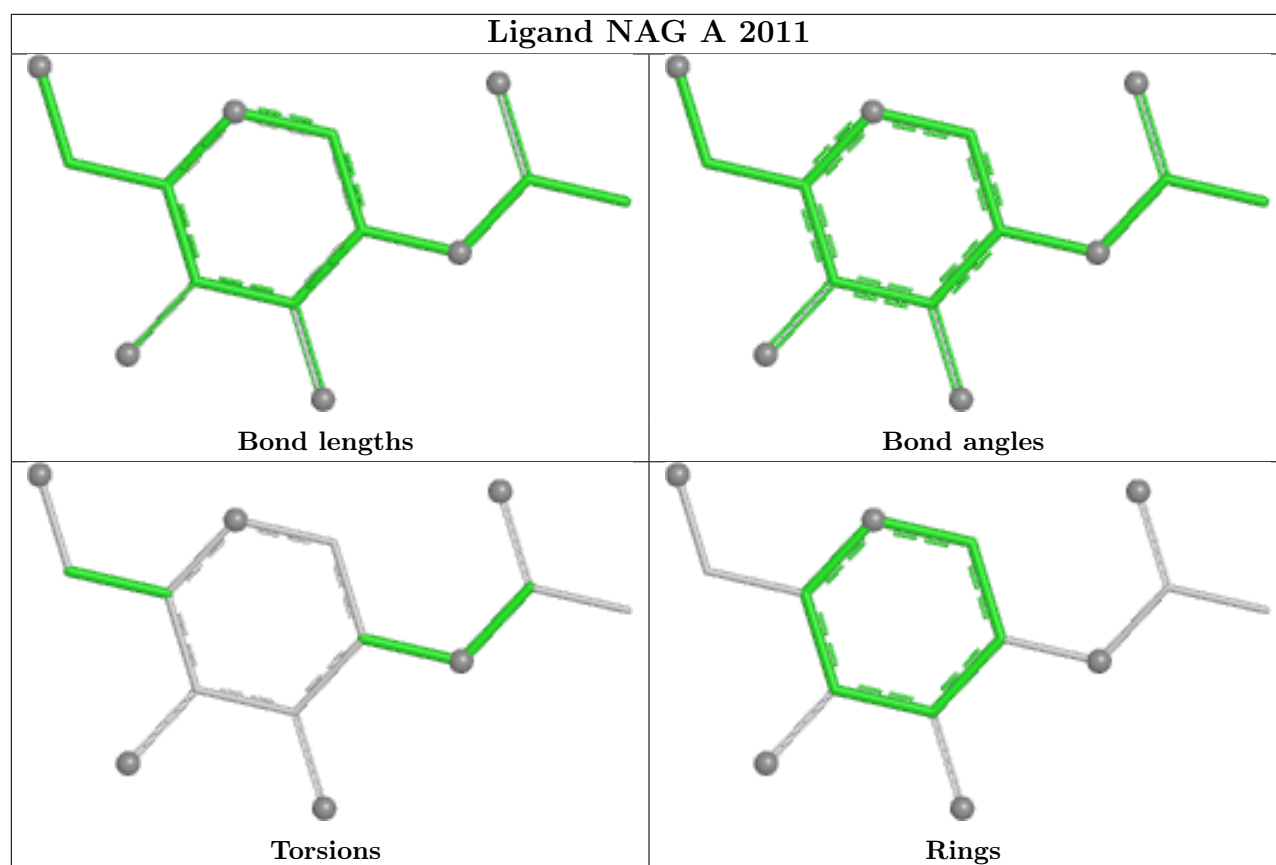


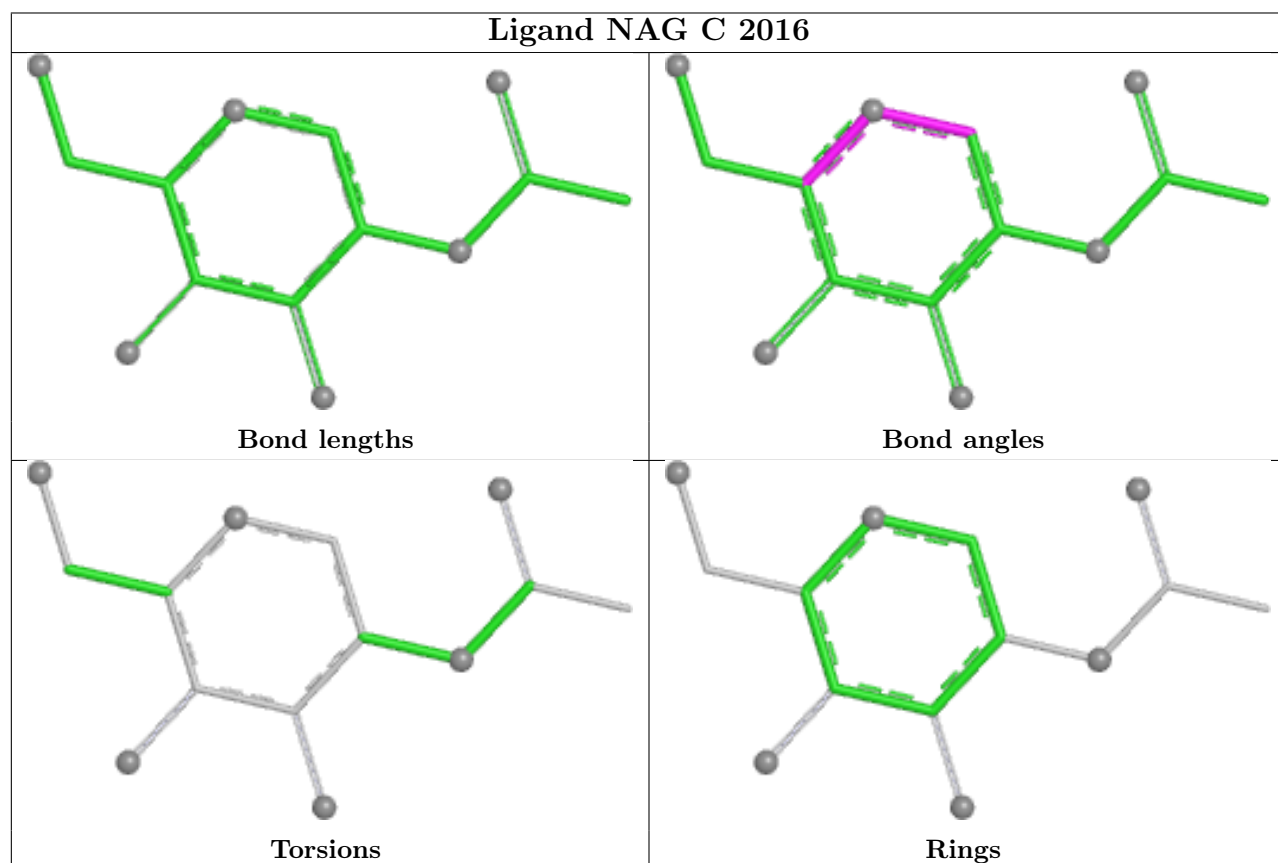
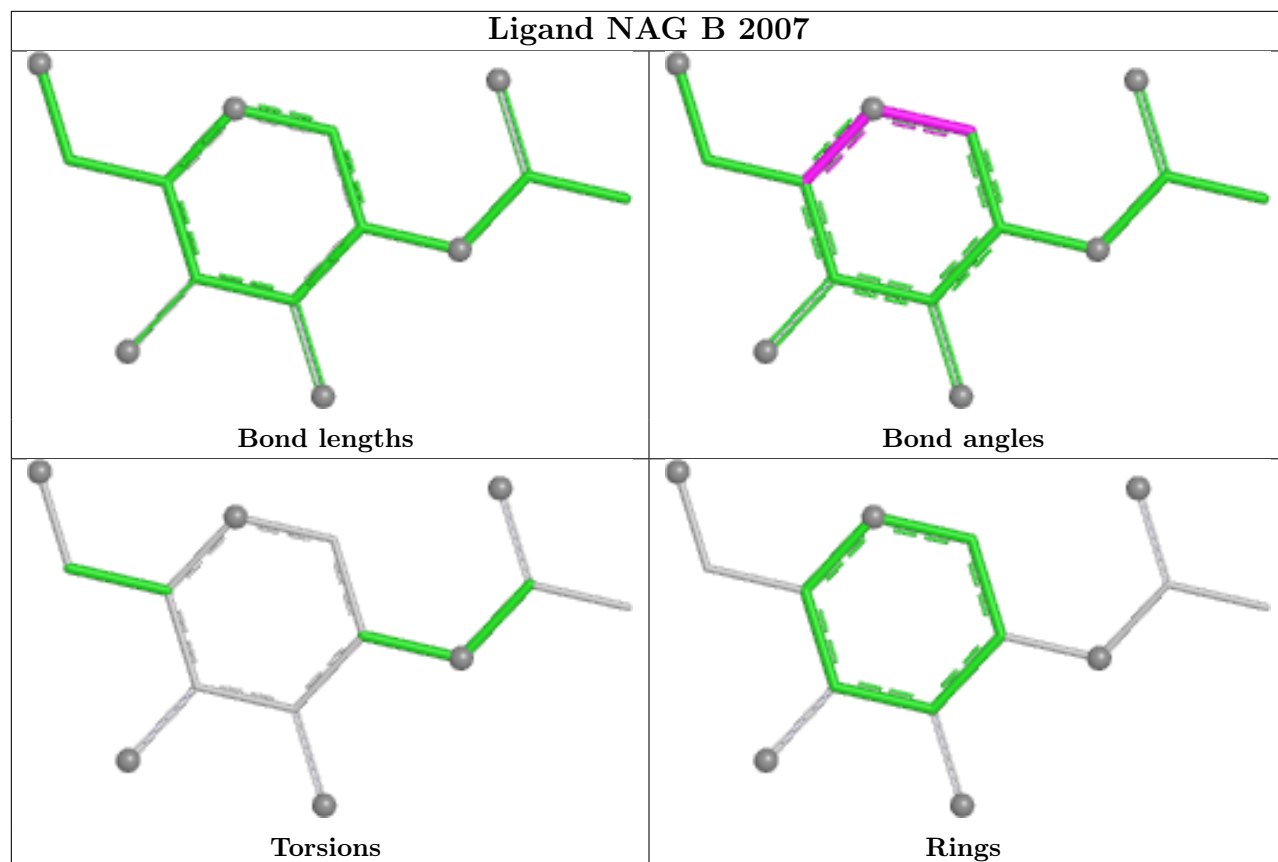
Ligand NAG C 2017



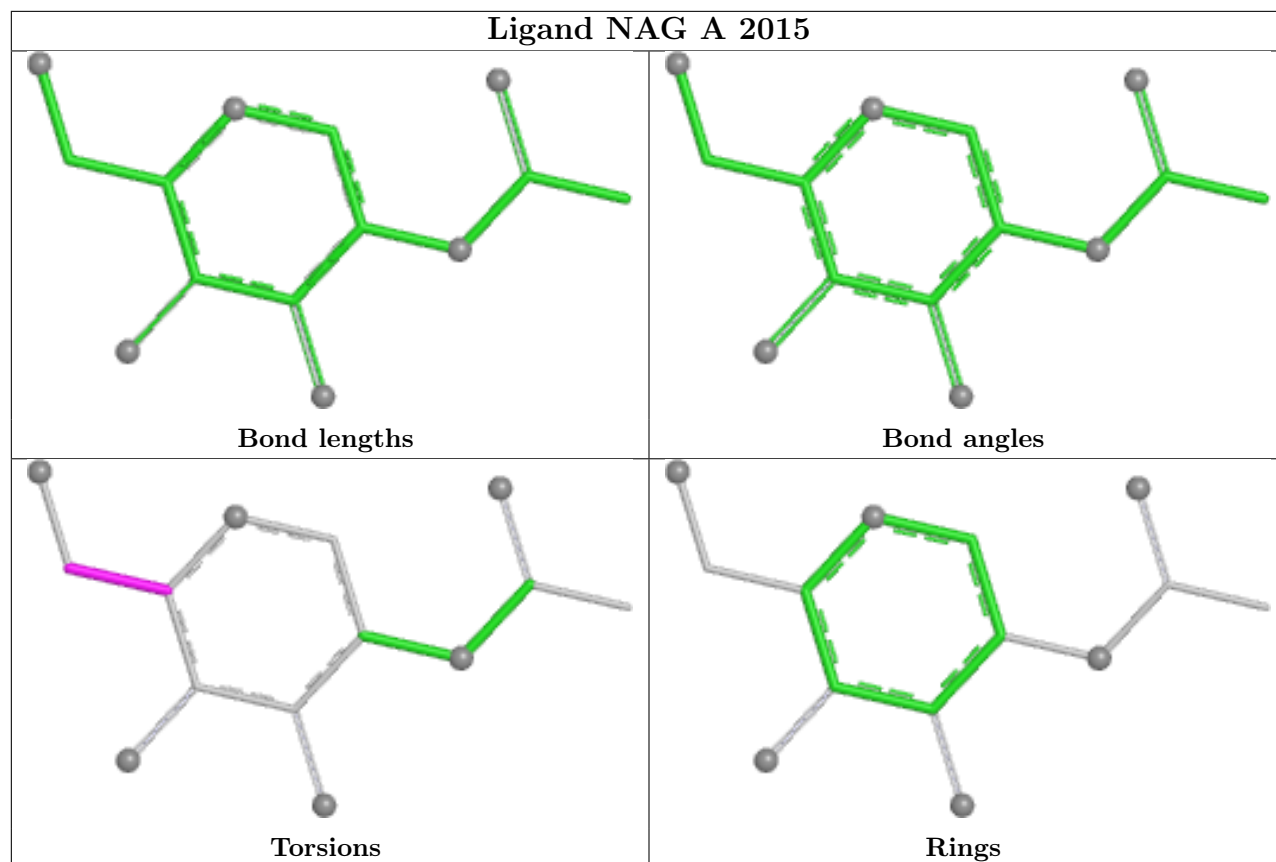
Ligand NAG B 2017



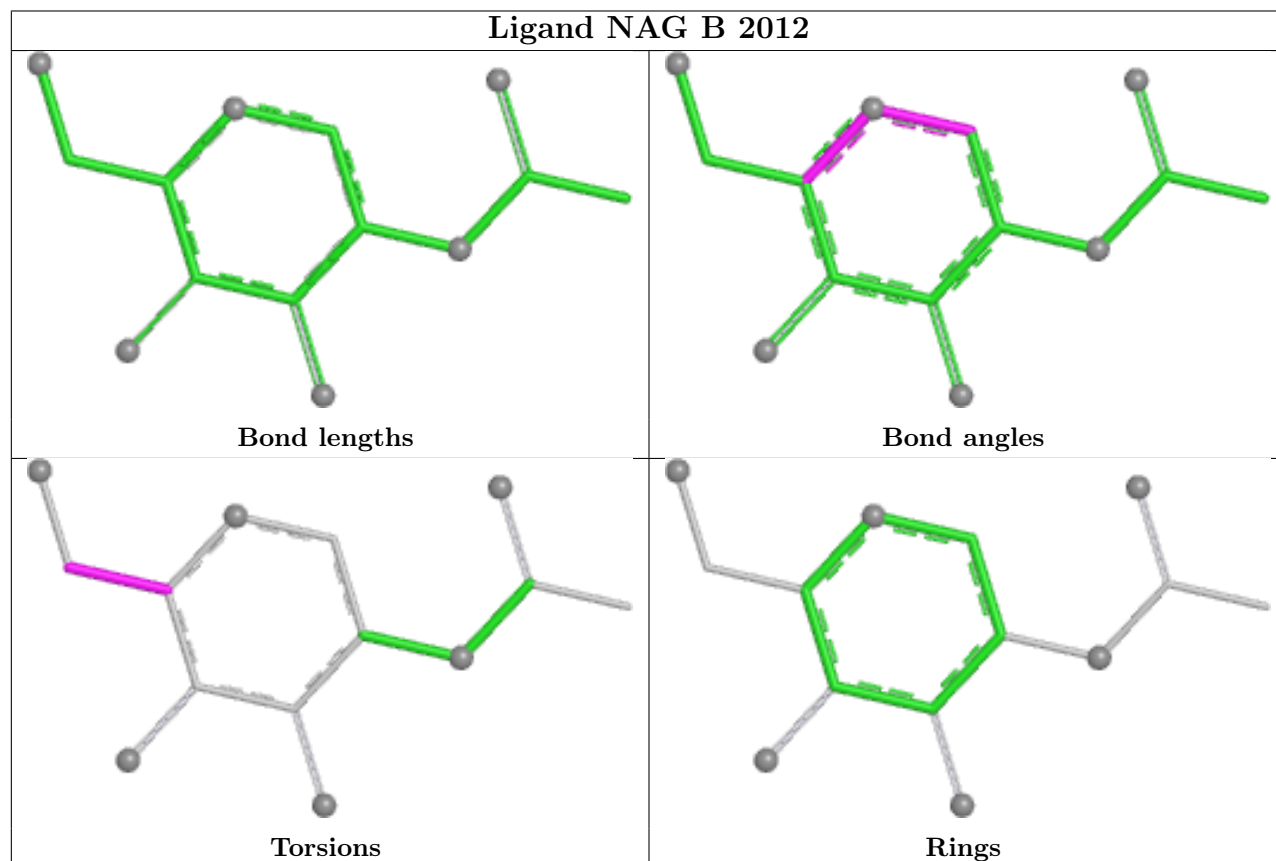




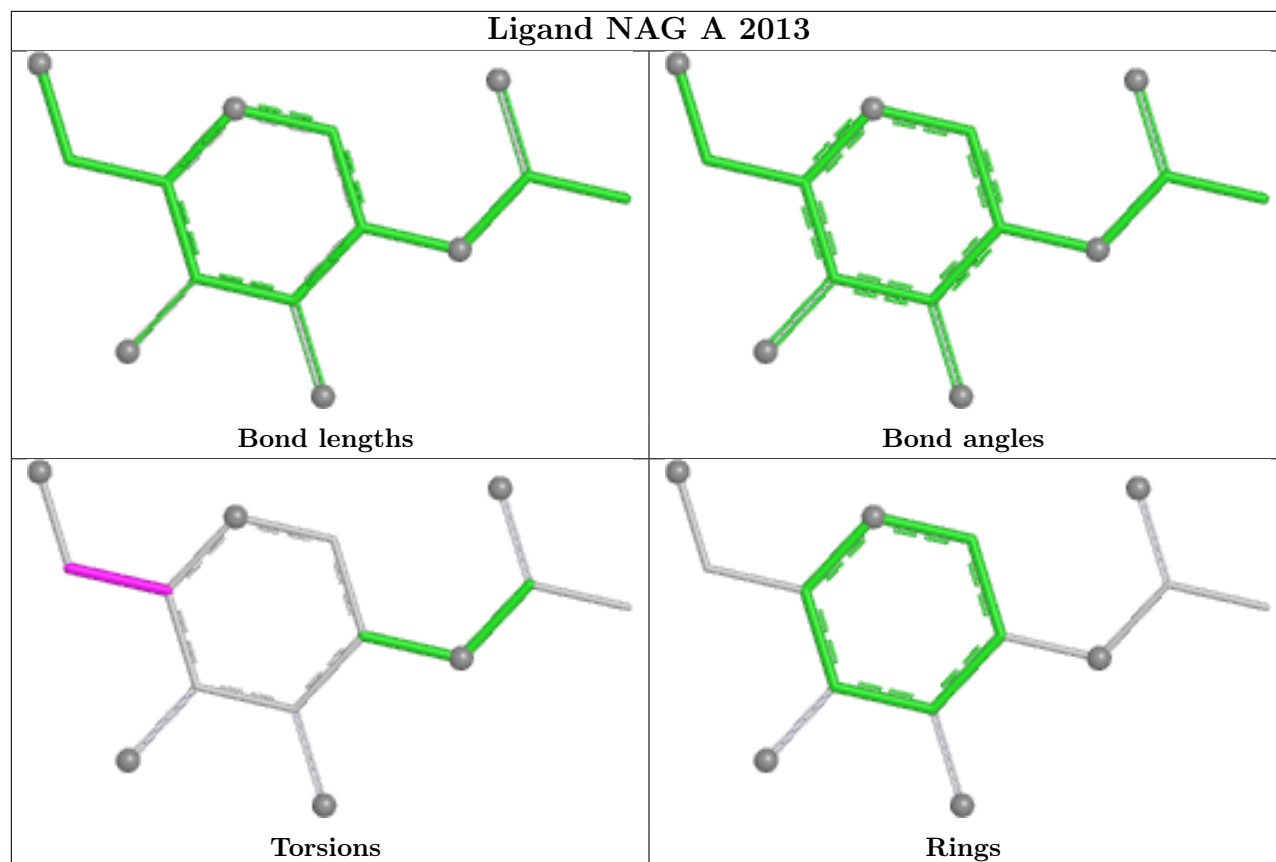
Ligand NAG A 2015



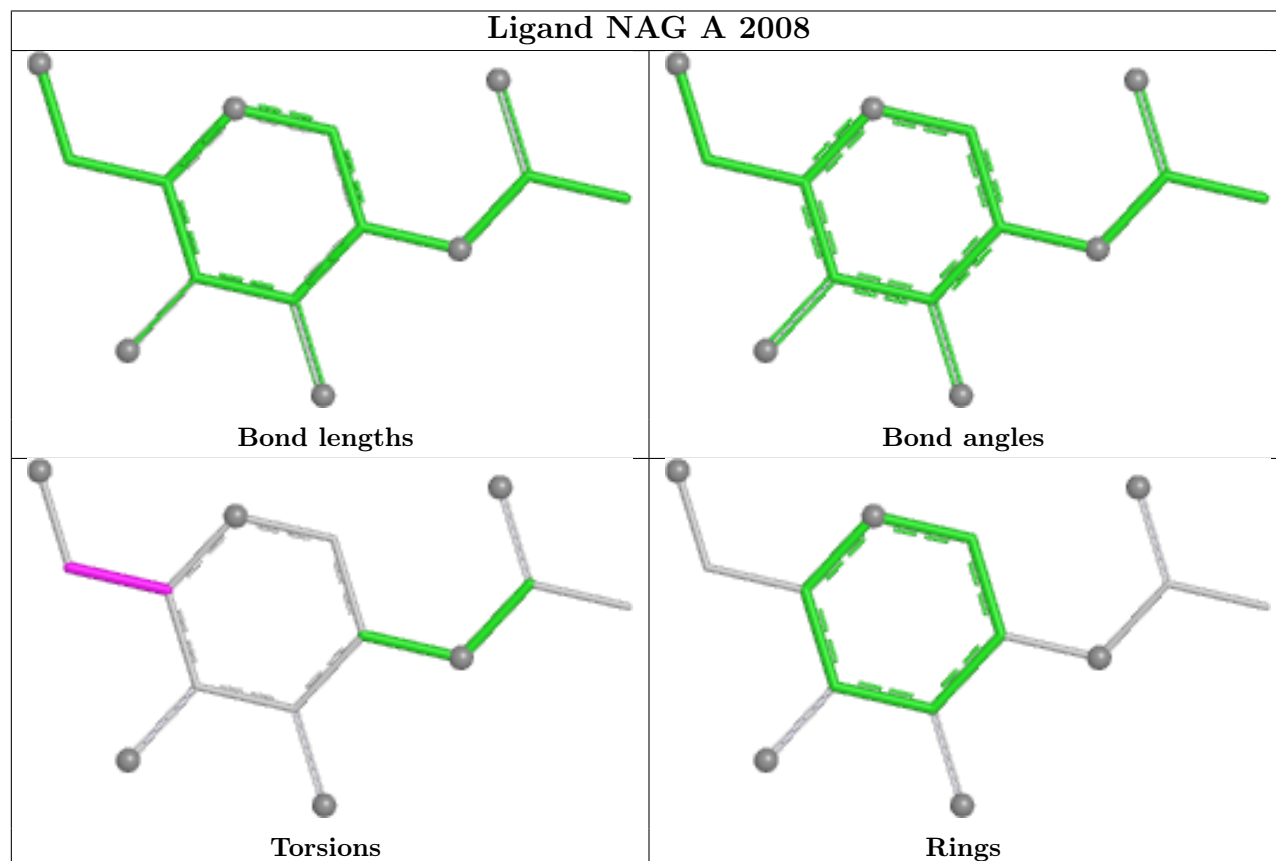
Ligand NAG B 2012

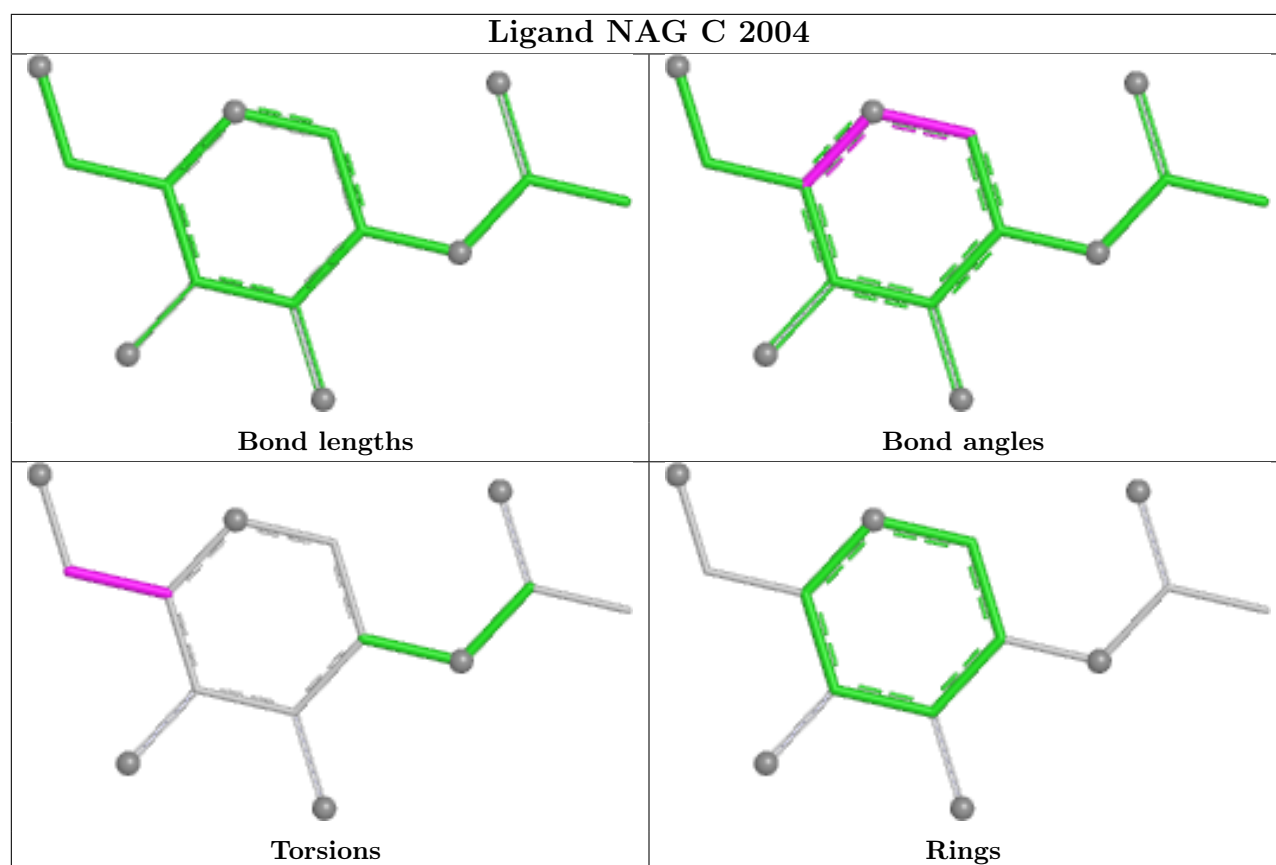


Ligand NAG A 2013



Ligand NAG A 2008





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.

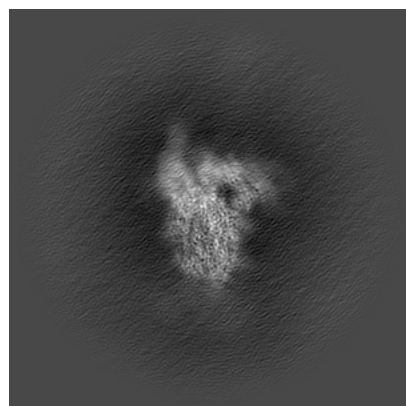
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38836. These allow visual inspection of the internal detail of the map and identification of artifacts.

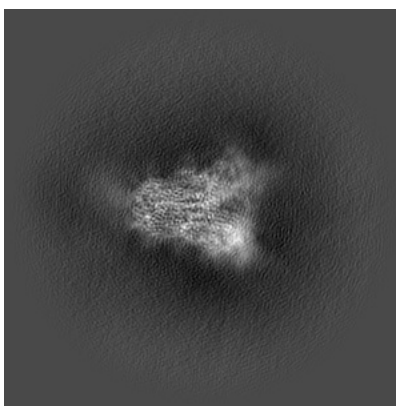
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

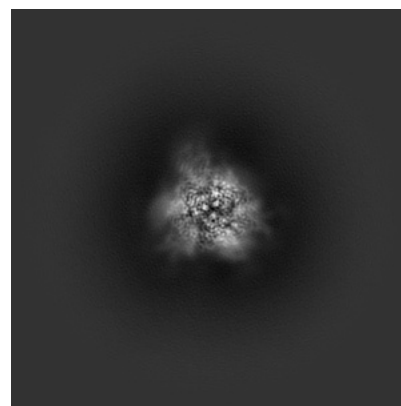
6.1.1 Primary map



X

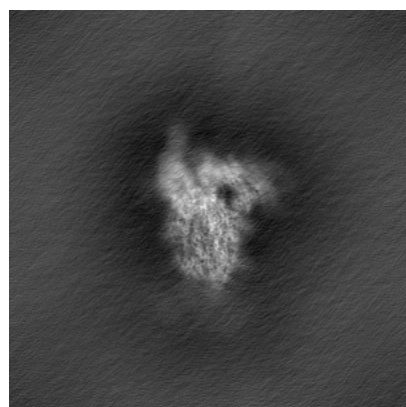


Y

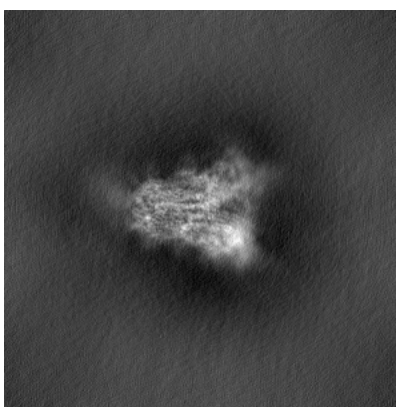


Z

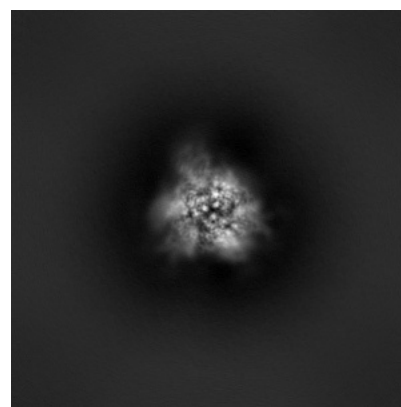
6.1.2 Raw map



X



Y

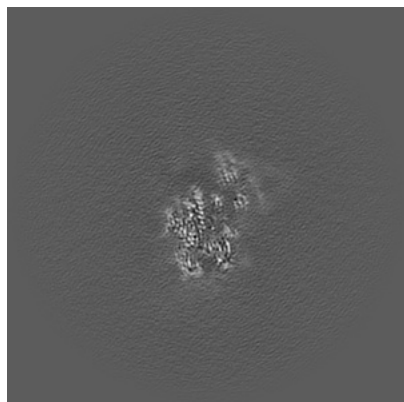


Z

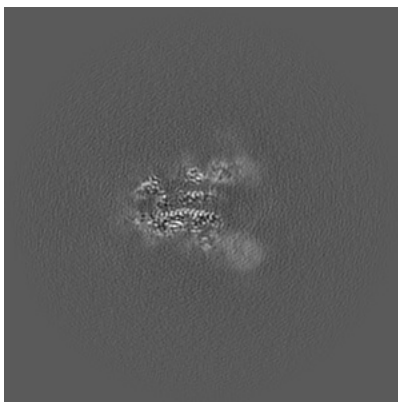
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

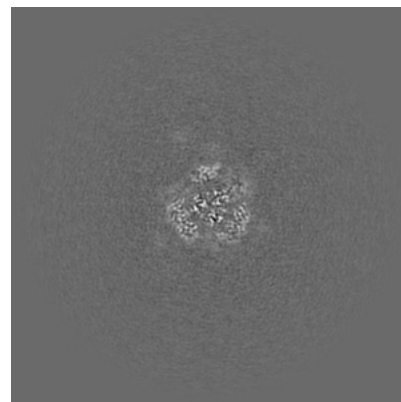
6.2.1 Primary map



X Index: 200

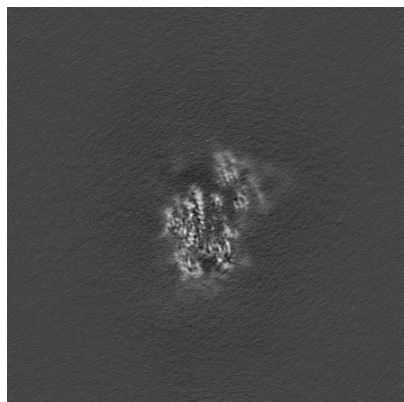


Y Index: 200

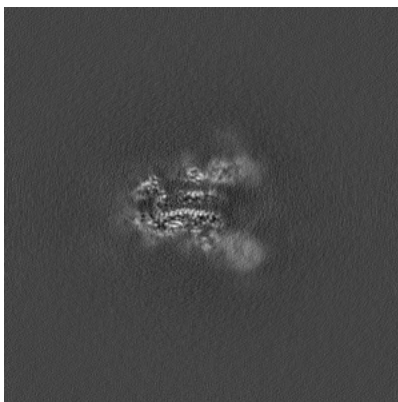


Z Index: 200

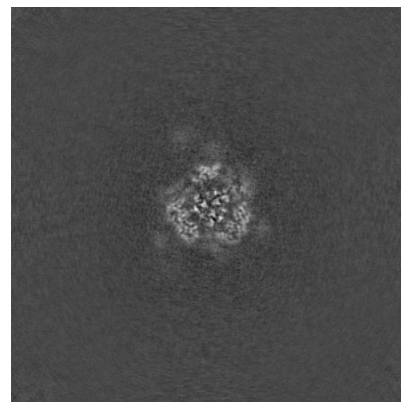
6.2.2 Raw map



X Index: 200



Y Index: 200

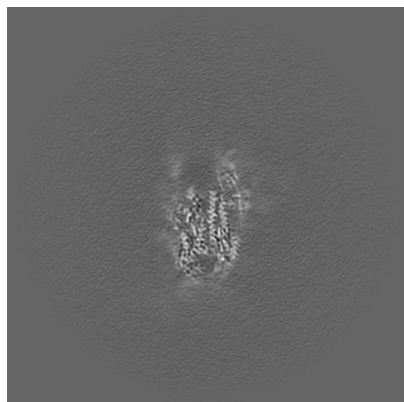


Z Index: 200

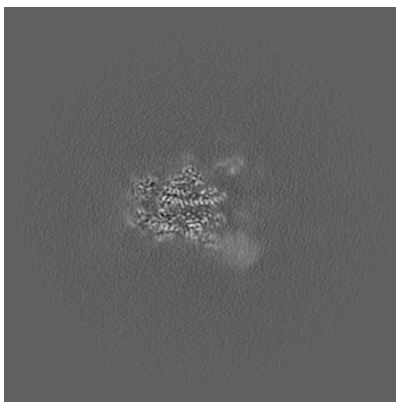
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

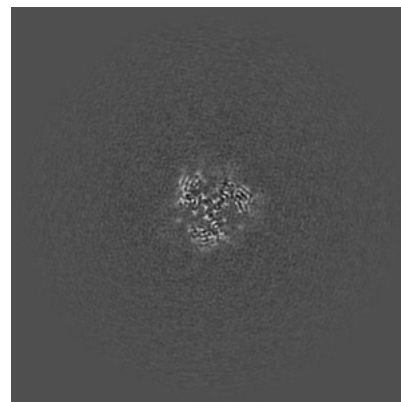
6.3.1 Primary map



X Index: 205

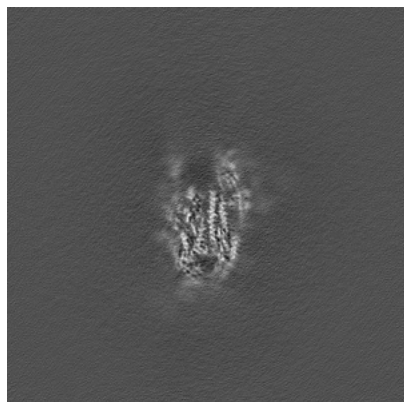


Y Index: 206

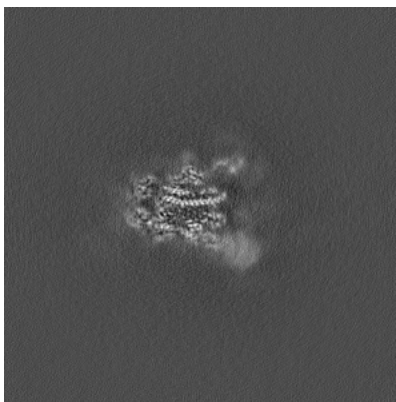


Z Index: 187

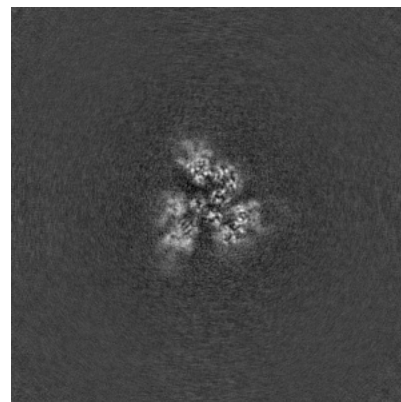
6.3.2 Raw map



X Index: 205



Y Index: 205

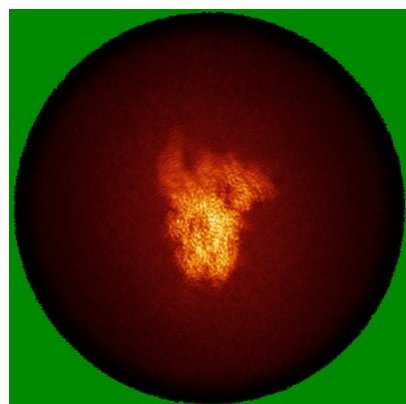


Z Index: 212

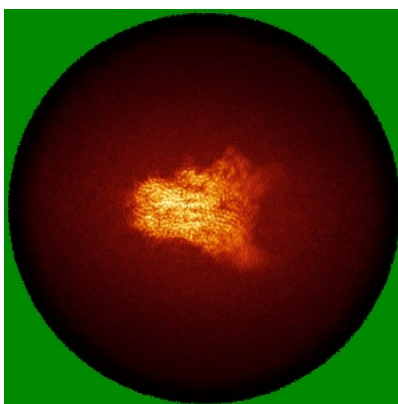
The images above show the largest variance slices of the map in three orthogonal directions.

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

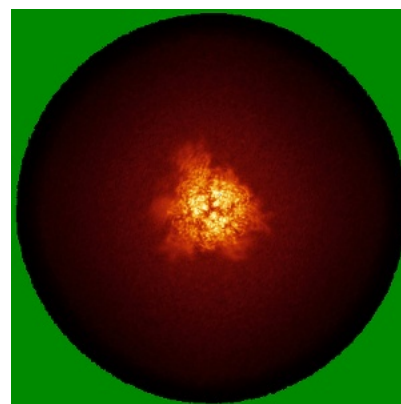
6.4.1 Primary map



X



Y

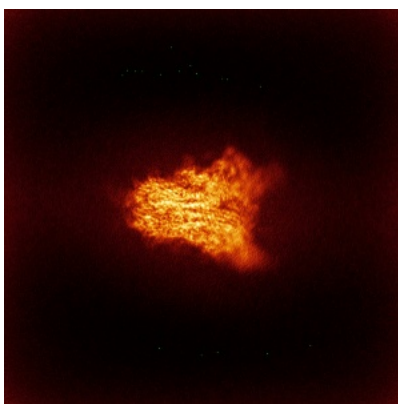


Z

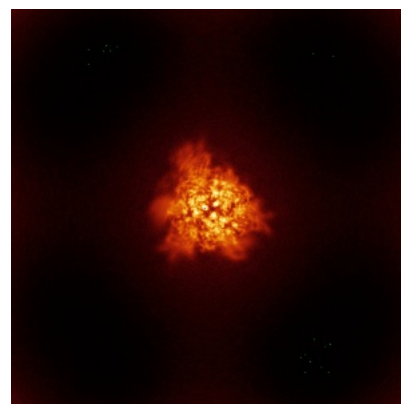
6.4.2 Raw map



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.

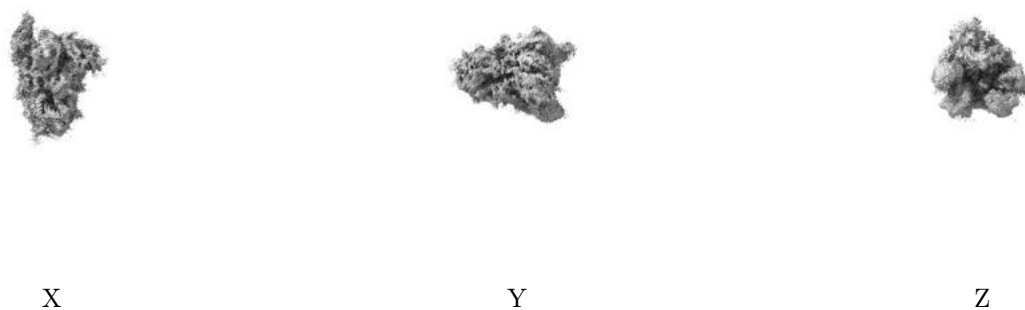
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.33. 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.

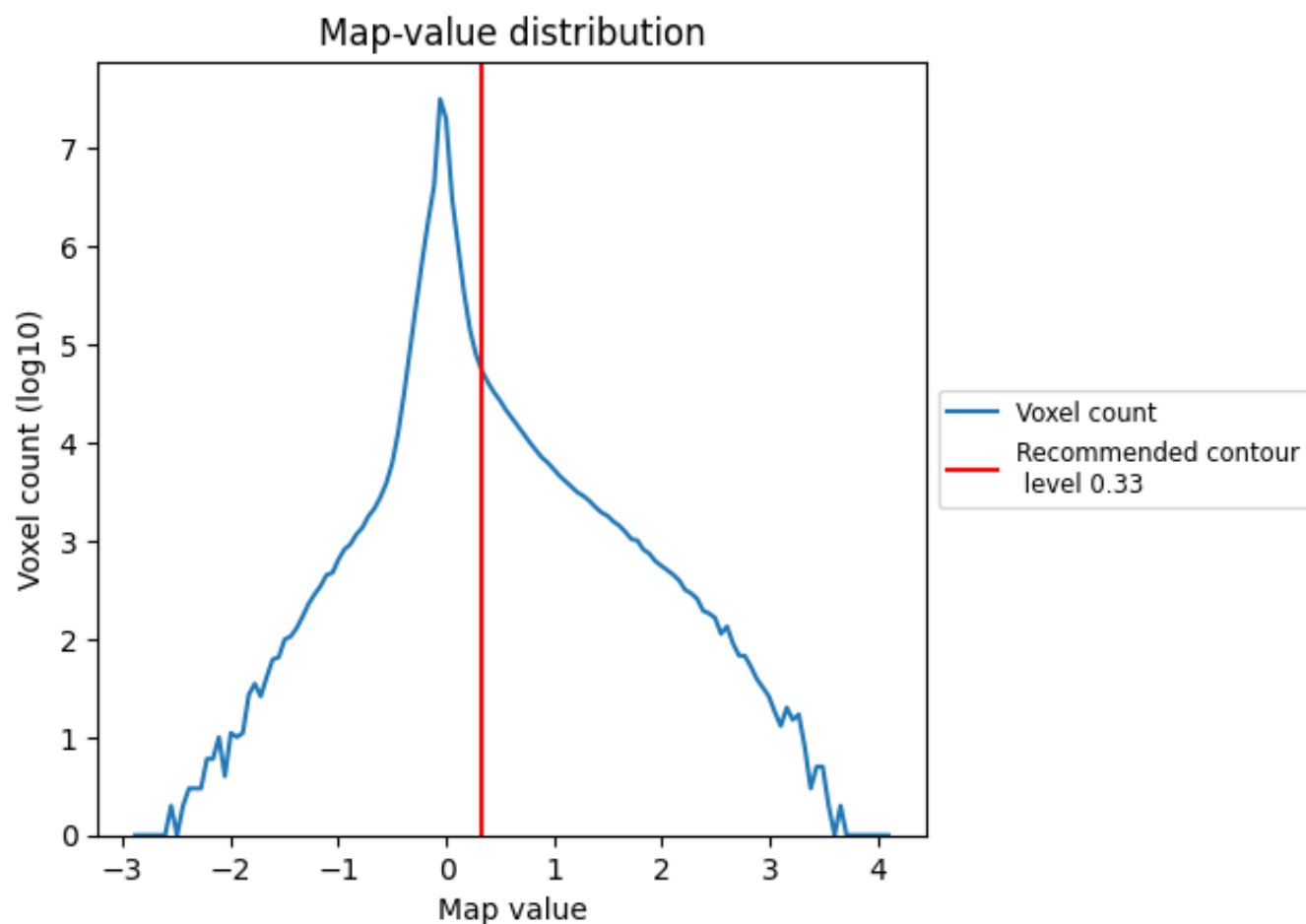
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

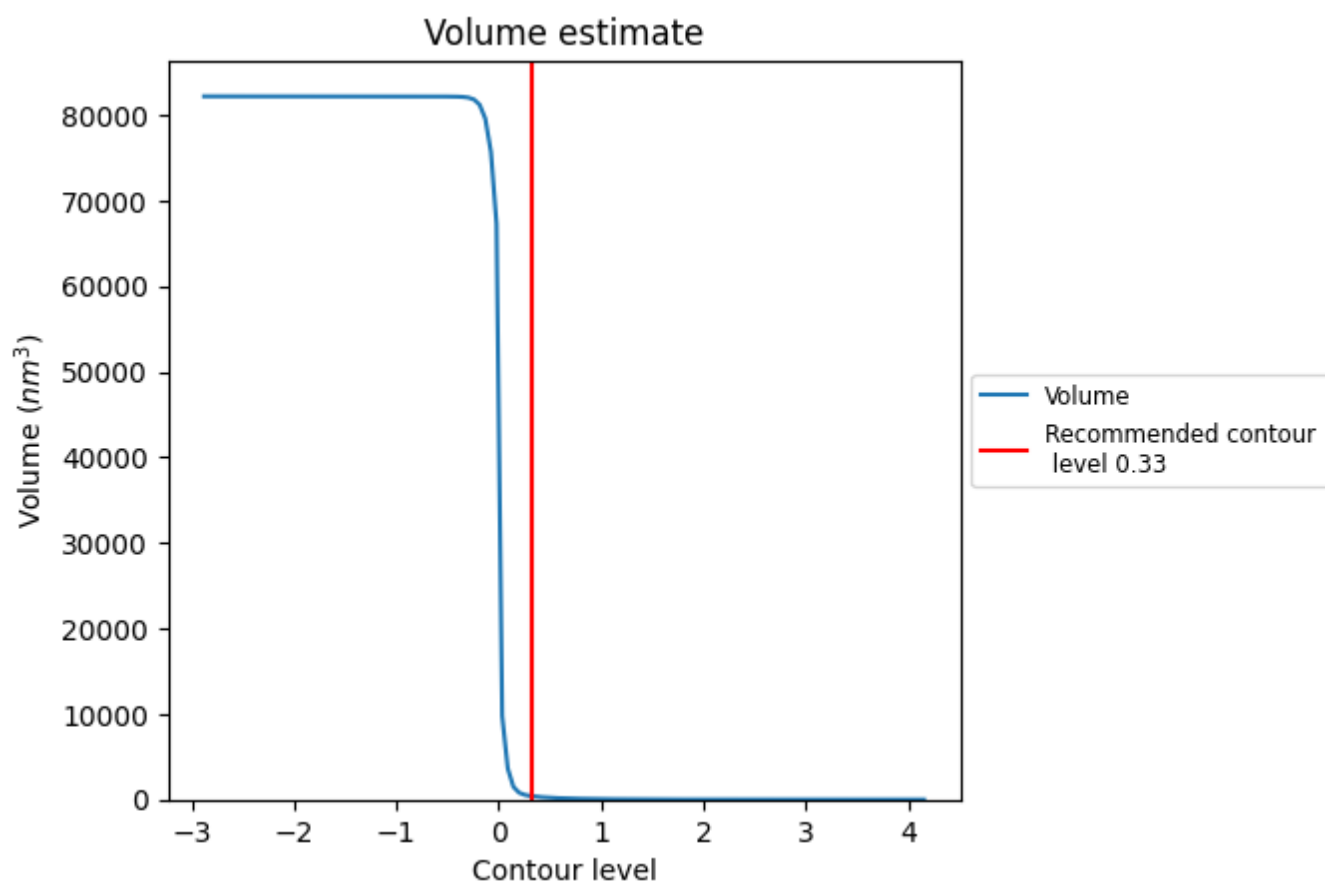
This section contains the results of statistical analysis of the map.

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.

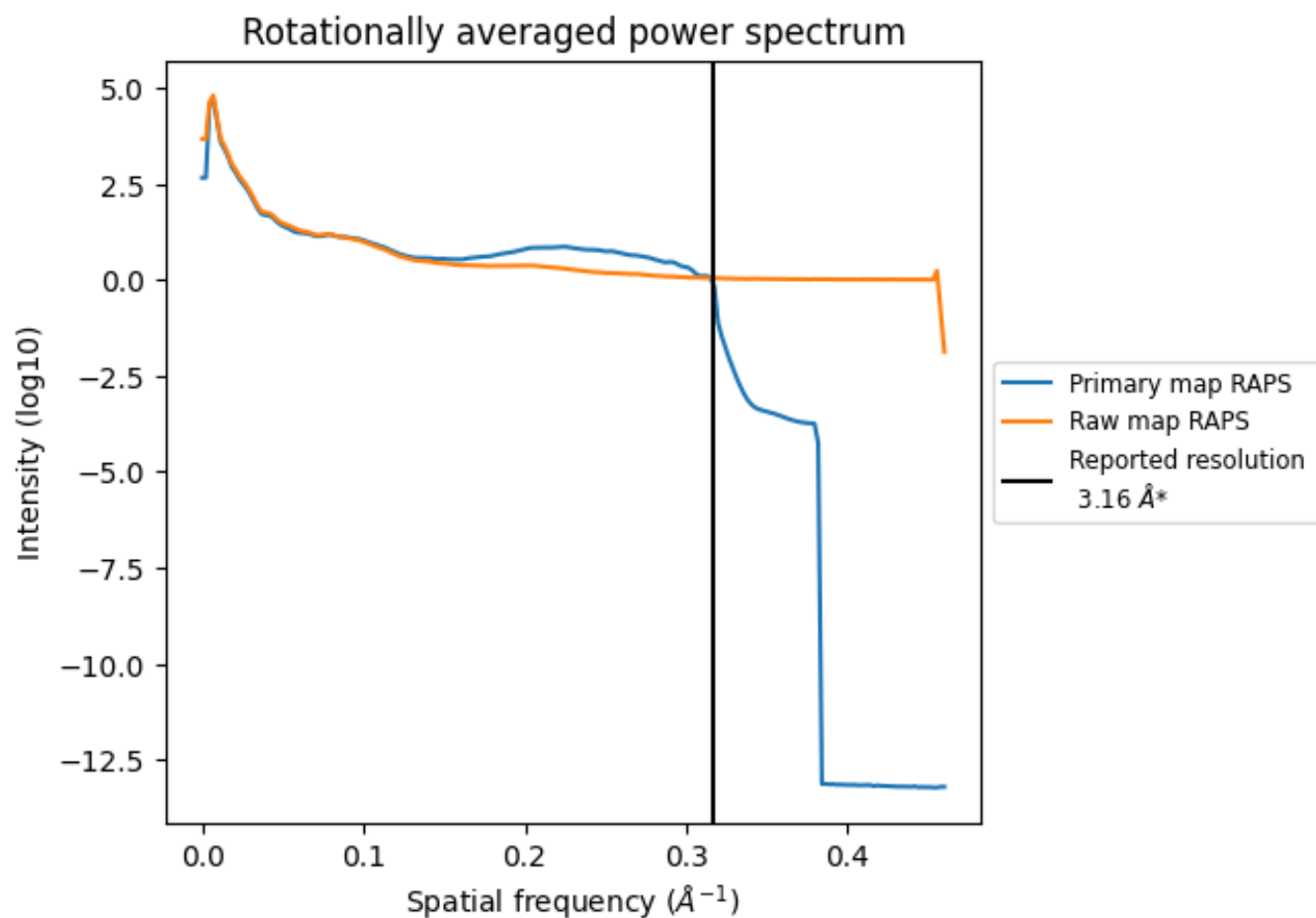
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 390 nm³; this corresponds to an approximate mass of 353 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 ⓘ

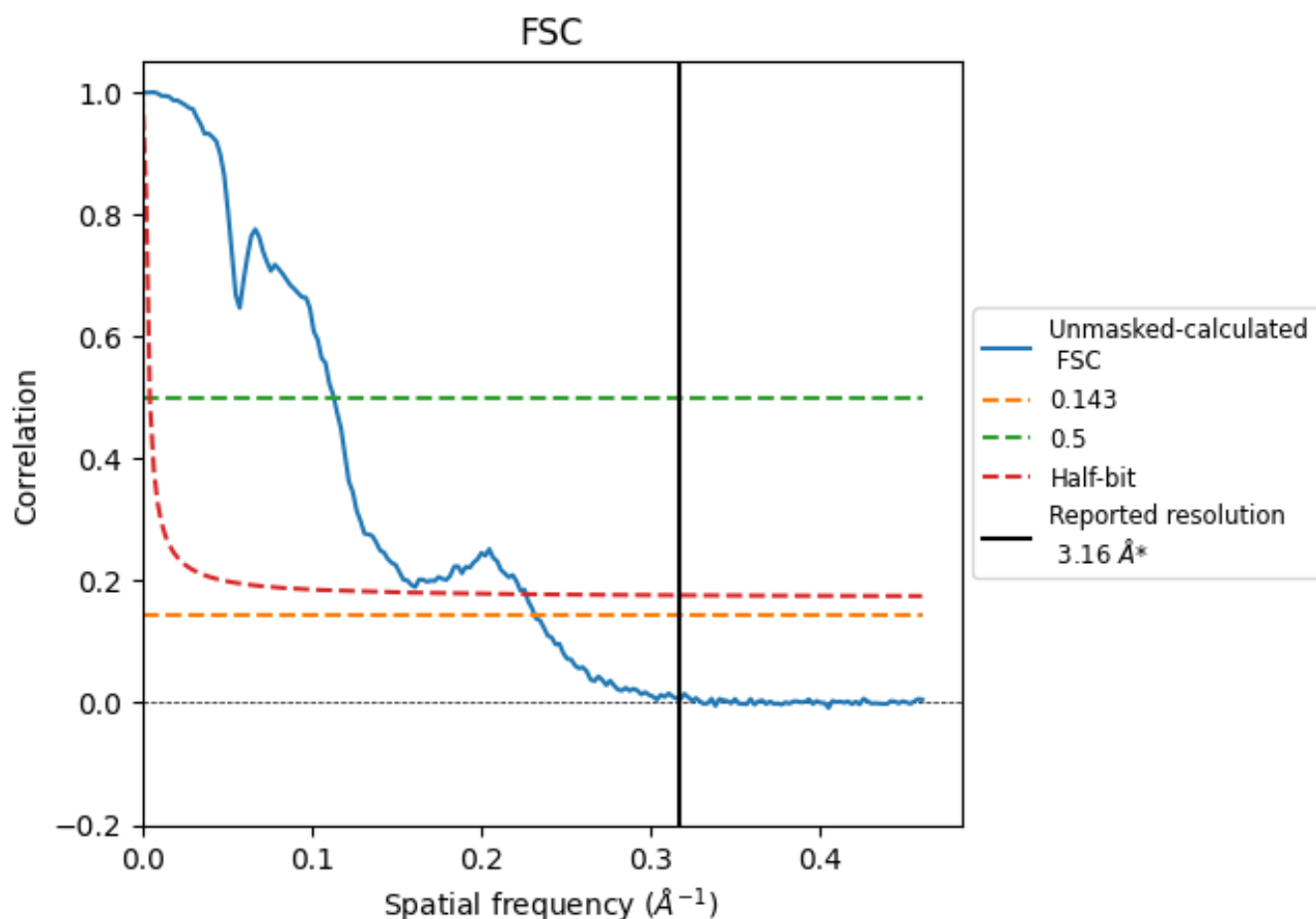


*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

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 0.316 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.32	8.85	4.42

*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 4.32 differs from the reported value 3.16 by more than 10 %

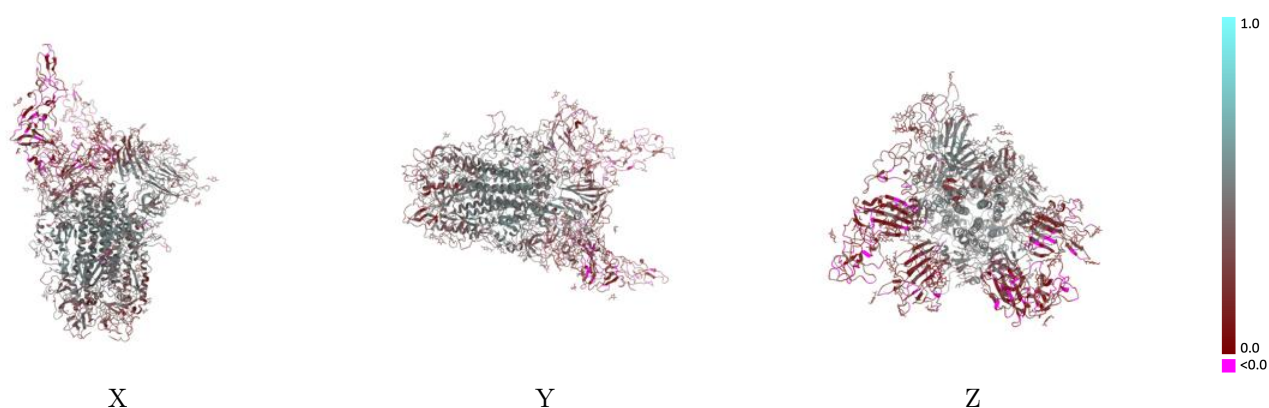
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-38836 and PDB model 8Y1H. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

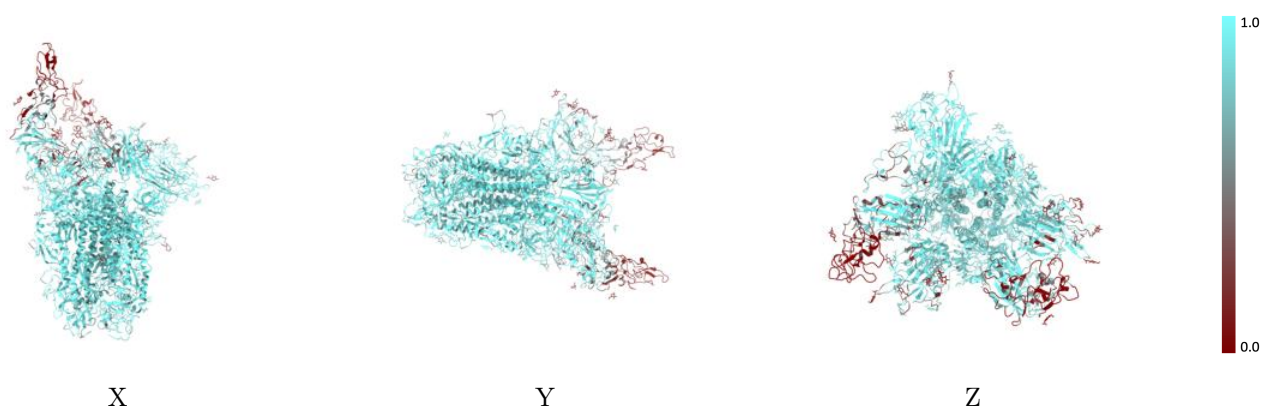
This section was not generated.

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



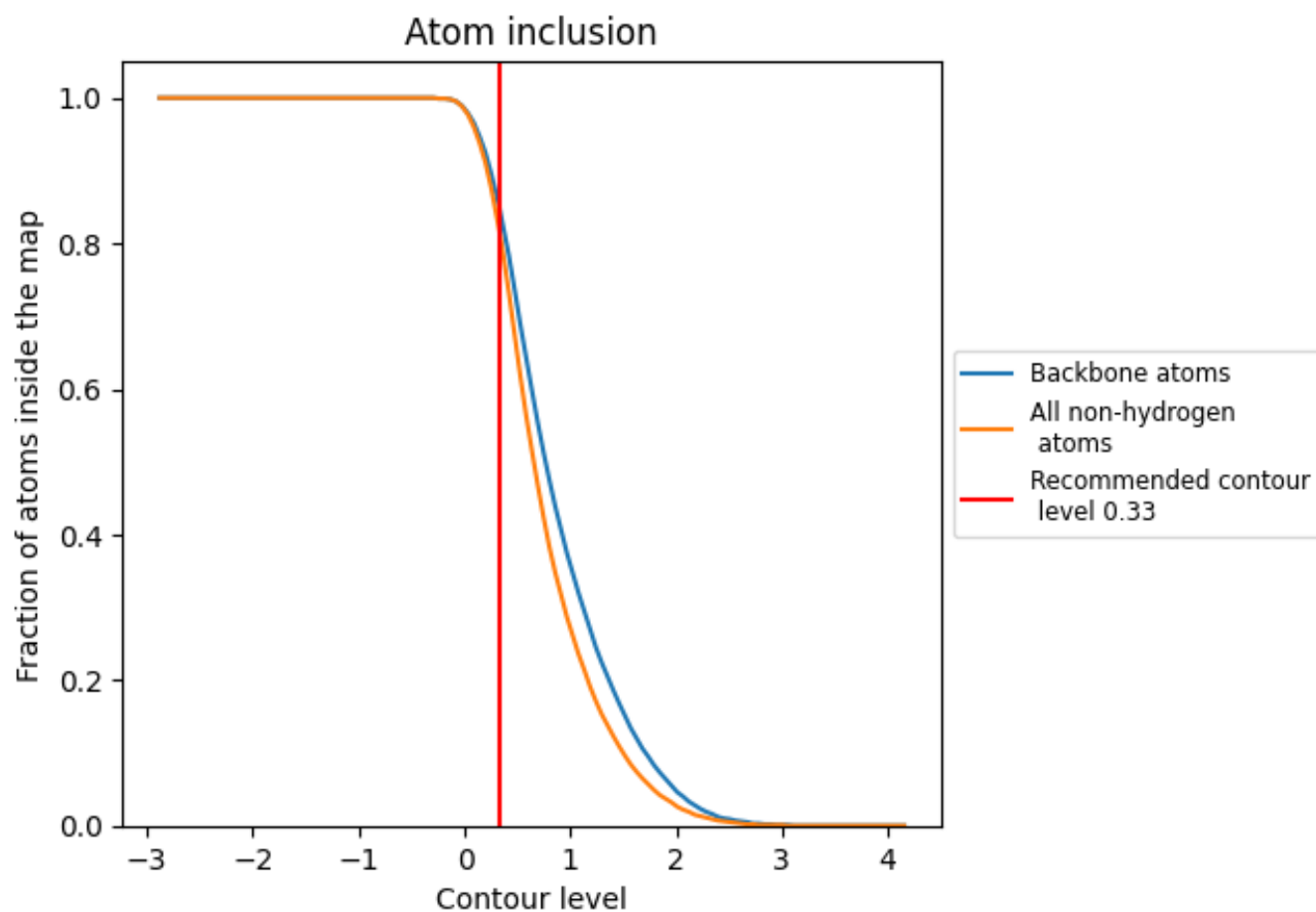
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.33).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8170	 0.3530
A	 0.8090	 0.3650
B	 0.7820	 0.3240
C	 0.8710	 0.3760
D	 0.2780	 0.1330
E	 0.5360	 0.2460
F	 0.6790	 0.1960
G	 0.9640	 0.3200
H	 0.9640	 0.3520
I	 0.3750	 0.1970
J	 0.5710	 0.1950
K	 0.7860	 0.4000
L	 0.2860	 0.2410
M	 0.7500	 0.2920
N	 0.8060	 0.2600
O	 0.8570	 0.3360
P	 0.3210	 0.3000
Q	 0.7500	 0.1790
R	 0.7140	 0.2580

