



## Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 03:17 PM JST

PDB ID : 7CYC  
EMDB ID : EMD-30496  
Title : Cryo-EM structures of Alphacoronavirus spike glycoprotein  
Authors : Song, X.; Shi, Y.; Ding, W.; Liu, Z.J.; Peng, G.  
Deposited on : 2020-09-03  
Resolution : 3.21 Å (reported)  
Based on initial model : 5SZS

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

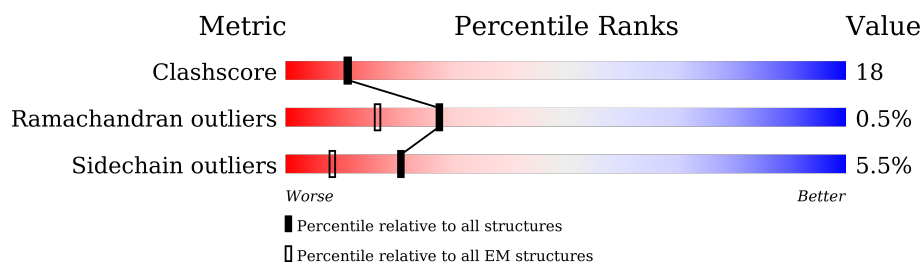
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.21 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1116	
1	B	1116	
1	C	1116	
2	D	7	
2	H	7	
2	L	7	
3	E	3	
3	G	3	

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Mol	Chain	Length	Quality of chain
3	I	3	
3	K	3	
3	M	3	
3	O	3	
4	F	2	
4	J	2	
4	N	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	1201	-	-	X	-
5	NAG	B	1201	-	-	X	-
5	NAG	C	1201	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22521 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

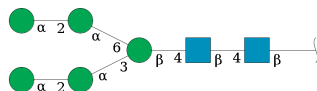
- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	959	Total	C	N	O	S	0	0
			7094	4483	1225	1349	37		
1	B	959	Total	C	N	O	S	0	0
			7094	4483	1225	1349	37		
1	C	959	Total	C	N	O	S	0	0
			7094	4483	1225	1349	37		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	642	MET	ARG	variant	UNP P15423
A	681	ARG	THR	variant	UNP P15423
A	765	ALA	VAL	variant	UNP P15423
A	775	SER	ALA	variant	UNP P15423
A	871	ILE	THR	variant	UNP P15423
A	937	LEU	ILE	variant	UNP P15423
A	971	ARG	THR	variant	UNP P15423
A	1005	ILE	MET	variant	UNP P15423
B	642	MET	ARG	variant	UNP P15423
B	681	ARG	THR	variant	UNP P15423
B	765	ALA	VAL	variant	UNP P15423
B	775	SER	ALA	variant	UNP P15423
B	871	ILE	THR	variant	UNP P15423
B	937	LEU	ILE	variant	UNP P15423
B	971	ARG	THR	variant	UNP P15423
B	1005	ILE	MET	variant	UNP P15423
C	642	MET	ARG	variant	UNP P15423
C	681	ARG	THR	variant	UNP P15423
C	765	ALA	VAL	variant	UNP P15423
C	775	SER	ALA	variant	UNP P15423
C	871	ILE	THR	variant	UNP P15423
C	937	LEU	ILE	variant	UNP P15423
C	971	ARG	THR	variant	UNP P15423
C	1005	ILE	MET	variant	UNP P15423

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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
2	D	7	Total	C	N	O	0	0
			83	46	2	35		
2	H	7	Total	C	N	O	0	0
			83	46	2	35		
2	L	7	Total	C	N	O	0	0
			83	46	2	35		

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



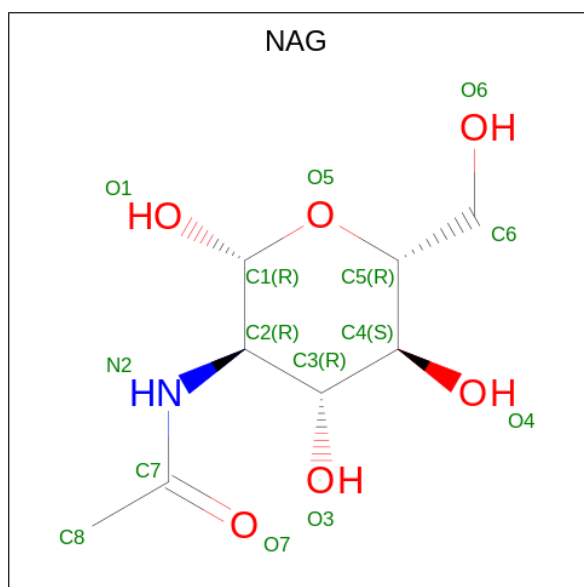
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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

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

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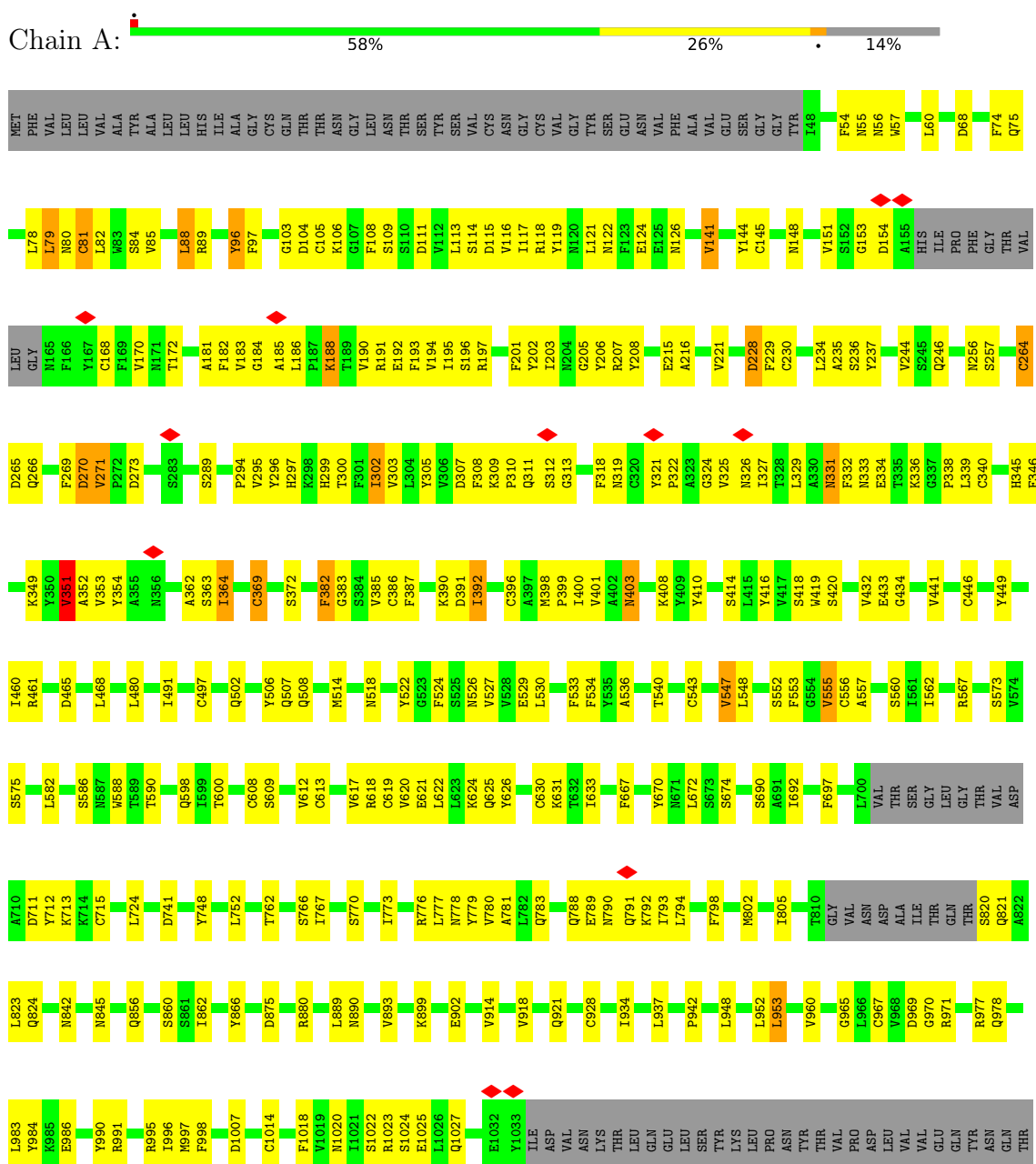
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5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



### 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 2:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -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



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



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



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



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



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





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

Chain O: 



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

Chain F: 



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

Chain J: 



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

Chain N: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36846	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	18000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	29.222	Depositor
Minimum map value	-10.273	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size (Å)	280.0, 280.0, 280.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/7246	0.63	0/9752
1	B	0.41	0/7246	0.63	0/9752
1	C	0.41	0/7246	0.63	0/9752
All	All	0.41	0/21738	0.63	0/29256

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	7094	0	6274	277	0
1	B	7094	0	6273	284	0
1	C	7094	0	6273	259	0
2	D	83	0	70	0	0
2	H	83	0	70	0	0
2	L	83	0	70	0	0
3	E	39	0	34	0	0
3	G	39	0	34	2	0
3	I	39	0	34	0	0
3	K	39	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	39	0	34	0	0
3	O	39	0	34	2	0
4	F	28	0	25	0	0
4	J	28	0	25	0	0
4	N	28	0	25	0	0
5	A	224	0	208	15	0
5	B	224	0	208	14	0
5	C	224	0	208	15	0
All	All	22521	0	19933	766	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (766) 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:230:CYS:SG	5:B:1202:NAG:H83	1.52	1.50
1:C:230:CYS:SG	5:C:1202:NAG:H83	1.52	1.49
1:A:230:CYS:SG	5:A:1202:NAG:H83	1.57	1.44
1:B:78:LEU:CD2	1:B:236:SER:HB2	1.65	1.27
1:A:78:LEU:CD2	1:A:236:SER:HB2	1.65	1.26
1:B:78:LEU:HD22	1:B:236:SER:CB	1.67	1.25
1:A:78:LEU:HD22	1:A:236:SER:CB	1.67	1.24
1:C:78:LEU:CD2	1:C:236:SER:HB2	1.65	1.24
1:C:78:LEU:HD22	1:C:236:SER:CB	1.67	1.23
1:B:79:LEU:HD11	1:B:108:PHE:CD1	1.80	1.16
1:A:79:LEU:HD11	1:A:108:PHE:CD1	1.81	1.15
1:C:79:LEU:HD11	1:C:108:PHE:CD1	1.81	1.14
1:B:122:ASN:ND2	1:B:230:CYS:SG	2.23	1.11
1:B:230:CYS:SG	5:B:1202:NAG:C8	2.38	1.11
1:C:230:CYS:SG	5:C:1202:NAG:C8	2.38	1.11
1:A:122:ASN:ND2	1:A:230:CYS:SG	2.23	1.10
1:C:122:ASN:ND2	1:C:230:CYS:SG	2.23	1.10
1:A:230:CYS:SG	5:A:1202:NAG:C8	2.41	1.08
1:B:79:LEU:HD23	1:B:79:LEU:H	1.19	1.06
1:C:68:ASP:HA	1:C:244:VAL:O	1.55	1.06
1:B:68:ASP:HA	1:B:244:VAL:O	1.55	1.05
1:A:68:ASP:HA	1:A:244:VAL:O	1.55	1.04
1:C:79:LEU:HD23	1:C:79:LEU:H	1.19	1.04
1:A:79:LEU:H	1:A:79:LEU:HD23	1.19	1.03
1:A:96:TYR:CD2	1:A:216:ALA:HB2	1.94	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD13	1:A:236:SER:O	1.58	1.02
1:C:78:LEU:HD13	1:C:236:SER:O	1.58	1.02
1:C:96:TYR:CD2	1:C:216:ALA:HB2	1.94	1.02
1:B:78:LEU:HD13	1:B:236:SER:O	1.58	1.01
1:B:96:TYR:CD2	1:B:216:ALA:HB2	1.94	1.01
1:A:122:ASN:HB2	1:A:230:CYS:SG	2.06	0.95
1:B:122:ASN:HB2	1:B:230:CYS:SG	2.06	0.95
1:C:122:ASN:HB2	1:C:230:CYS:SG	2.06	0.95
1:A:122:ASN:CB	1:A:230:CYS:SG	2.57	0.92
1:C:122:ASN:CB	1:C:230:CYS:SG	2.57	0.92
1:B:122:ASN:CB	1:B:230:CYS:SG	2.57	0.92
1:C:82:LEU:HB3	1:C:104:ASP:O	1.72	0.90
1:A:713:LYS:HE2	1:B:534:PHE:CE1	2.07	0.89
1:B:82:LEU:HB3	1:B:104:ASP:O	1.72	0.88
1:A:82:LEU:HB3	1:A:104:ASP:O	1.72	0.88
1:A:713:LYS:HE2	1:B:534:PHE:HE1	1.38	0.87
1:C:80:ASN:O	1:C:109:SER:HB3	1.75	0.86
1:A:80:ASN:O	1:A:109:SER:HB3	1.76	0.86
1:B:80:ASN:O	1:B:109:SER:HB3	1.75	0.86
1:B:300:THR:OG1	1:B:346:PHE:CB	2.24	0.85
1:C:300:THR:OG1	1:C:346:PHE:CB	2.24	0.85
1:C:78:LEU:HD13	1:C:236:SER:C	1.96	0.85
1:A:84:SER:HA	1:A:103:GLY:HA3	1.58	0.85
1:A:300:THR:OG1	1:A:346:PHE:CB	2.24	0.84
1:B:78:LEU:HD13	1:B:236:SER:C	1.96	0.84
1:A:78:LEU:HD13	1:A:236:SER:C	1.96	0.84
1:B:84:SER:HA	1:B:103:GLY:HA3	1.58	0.84
1:A:465:ASP:HB2	1:A:491:ILE:HD11	1.60	0.83
1:C:84:SER:HA	1:C:103:GLY:HA3	1.58	0.83
1:B:465:ASP:HB2	1:B:491:ILE:HD11	1.60	0.81
1:C:465:ASP:HB2	1:C:491:ILE:HD11	1.60	0.81
1:A:977:ARG:NH2	1:C:1007:ASP:OD1	2.14	0.81
1:A:96:TYR:CG	1:A:216:ALA:HB2	2.16	0.80
1:C:96:TYR:CG	1:C:216:ALA:HB2	2.16	0.80
1:B:96:TYR:CG	1:B:216:ALA:HB2	2.16	0.80
1:B:96:TYR:CE2	1:B:216:ALA:HB2	2.17	0.80
1:A:300:THR:OG1	1:A:346:PHE:HB3	1.82	0.80
1:A:96:TYR:CE2	1:A:216:ALA:HB2	2.17	0.79
1:A:575:SER:OG	1:A:995:ARG:HD2	1.83	0.79
1:C:575:SER:OG	1:C:995:ARG:HD2	1.83	0.79
1:C:96:TYR:CE2	1:C:216:ALA:HB2	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:THR:OG1	1:C:346:PHE:HB3	1.82	0.78
1:B:897:LEU:HD13	1:C:839:GLN:HE22	1.47	0.78
1:B:575:SER:OG	1:B:995:ARG:HD2	1.83	0.77
1:B:300:THR:OG1	1:B:346:PHE:HB3	1.82	0.77
1:A:340:CYS:HB2	1:A:386:CYS:SG	2.26	0.75
1:A:534:PHE:CE1	1:C:713:LYS:HE2	2.22	0.75
1:C:340:CYS:HB2	1:C:386:CYS:SG	2.26	0.75
1:B:340:CYS:HB2	1:B:386:CYS:SG	2.26	0.74
1:A:182:PHE:HB2	1:B:296:TYR:HB2	1.70	0.74
1:A:96:TYR:CD2	5:A:1201:NAG:H83	2.22	0.74
1:C:79:LEU:H	1:C:79:LEU:CD2	1.97	0.74
1:C:79:LEU:HD23	1:C:79:LEU:N	2.01	0.74
1:C:96:TYR:CD2	5:C:1201:NAG:H83	2.23	0.73
1:B:96:TYR:CD2	5:B:1201:NAG:H83	2.23	0.72
1:B:56:ASN:OD1	1:B:191:ARG:NH2	2.22	0.72
1:A:56:ASN:OD1	1:A:191:ARG:NH2	2.22	0.72
1:C:56:ASN:OD1	1:C:191:ARG:NH2	2.22	0.72
1:C:983:LEU:HD11	1:C:990:TYR:HB3	1.72	0.72
1:B:79:LEU:H	1:B:79:LEU:CD2	1.97	0.72
1:A:631:LYS:HE2	1:B:266:GLN:HA	1.72	0.71
1:A:1007:ASP:OD1	1:B:977:ARG:NH2	2.23	0.71
1:B:983:LEU:HD11	1:B:990:TYR:HB3	1.72	0.71
1:A:78:LEU:HB2	1:A:236:SER:H	1.56	0.70
1:A:185:ALA:HB2	1:B:294:PRO:HB2	1.74	0.70
1:A:79:LEU:H	1:A:79:LEU:CD2	1.97	0.70
1:A:983:LEU:HD11	1:A:990:TYR:HB3	1.72	0.70
1:A:79:LEU:HD23	1:A:79:LEU:N	2.01	0.70
1:B:79:LEU:HD23	1:B:79:LEU:N	2.01	0.70
1:C:788:GLN:O	1:C:792:LYS:NZ	2.24	0.70
1:B:1023:ARG:O	1:B:1027:GLN:NE2	2.25	0.70
1:B:78:LEU:HB2	1:B:236:SER:H	1.56	0.70
1:A:319:ASN:HB2	1:A:410:TYR:HB2	1.73	0.70
1:A:1023:ARG:O	1:A:1027:GLN:NE2	2.25	0.70
1:C:1023:ARG:O	1:C:1027:GLN:NE2	2.24	0.70
1:B:598:GLN:NE2	1:B:600:THR:O	2.25	0.70
1:A:788:GLN:O	1:A:792:LYS:NZ	2.24	0.69
1:B:788:GLN:O	1:B:792:LYS:NZ	2.24	0.69
1:C:78:LEU:HB2	1:C:236:SER:H	1.56	0.69
1:C:776:ARG:HB3	1:C:921:GLN:OE1	1.92	0.69
1:A:534:PHE:HE1	1:C:713:LYS:HE2	1.56	0.69
1:C:598:GLN:NE2	1:C:600:THR:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ASP:N	1:A:228:ASP:OD1	2.25	0.69
1:A:598:GLN:NE2	1:A:600:THR:O	2.25	0.69
1:A:953:LEU:HD21	3:G:1:NAG:H3	1.75	0.69
1:C:228:ASP:OD1	1:C:228:ASP:N	2.25	0.69
1:C:319:ASN:HB2	1:C:410:TYR:HB2	1.73	0.69
1:A:182:PHE:HB2	1:B:296:TYR:HD2	1.58	0.68
1:A:776:ARG:HB3	1:A:921:GLN:OE1	1.93	0.68
1:B:319:ASN:HB2	1:B:410:TYR:HB2	1.74	0.68
1:B:776:ARG:HB3	1:B:921:GLN:OE1	1.93	0.68
1:A:184:GLY:HA3	1:B:295:VAL:HA	1.76	0.68
1:A:266:GLN:HA	1:C:631:LYS:HE2	1.76	0.67
1:A:300:THR:OG1	1:A:346:PHE:HB2	1.93	0.67
1:C:300:THR:OG1	1:C:346:PHE:HB2	1.94	0.67
1:C:588:TRP:CH2	1:C:997:MET:HG2	2.30	0.67
1:B:228:ASP:OD1	1:B:228:ASP:N	2.26	0.67
1:B:588:TRP:CH2	1:B:997:MET:HG2	2.30	0.67
1:A:296:TYR:HD2	1:C:182:PHE:HB2	1.58	0.66
1:A:588:TRP:CH2	1:A:997:MET:HG2	2.30	0.66
1:B:85:VAL:HG12	1:B:88:LEU:HB3	1.78	0.66
1:B:300:THR:OG1	1:B:346:PHE:HB2	1.93	0.66
1:A:777:LEU:HD22	1:A:783:GLN:HB2	1.78	0.66
1:C:119:TYR:HB2	1:C:193:PHE:HB3	1.77	0.66
1:C:124:GLU:OE2	1:C:126:ASN:ND2	2.28	0.66
1:B:119:TYR:HB2	1:B:193:PHE:HB3	1.77	0.66
1:B:124:GLU:OE2	1:B:126:ASN:ND2	2.28	0.66
1:C:777:LEU:HD22	1:C:783:GLN:HB2	1.78	0.66
1:A:96:TYR:CD1	5:A:1201:NAG:H82	2.31	0.65
1:A:119:TYR:HB2	1:A:193:PHE:HB3	1.77	0.65
1:A:124:GLU:OE2	1:A:126:ASN:ND2	2.28	0.65
1:C:85:VAL:HG12	1:C:88:LEU:HB3	1.78	0.65
1:B:622:LEU:HD21	1:B:875:ASP:HB3	1.78	0.65
1:B:777:LEU:HD22	1:B:783:GLN:HB2	1.78	0.65
1:C:80:ASN:C	1:C:109:SER:HB3	2.17	0.65
1:C:622:LEU:HD21	1:C:875:ASP:HB3	1.78	0.64
1:A:622:LEU:HD21	1:A:875:ASP:HB3	1.78	0.64
1:B:1007:ASP:OD1	1:C:977:ARG:NH2	2.30	0.64
1:A:80:ASN:C	1:A:109:SER:HB3	2.17	0.64
1:A:85:VAL:HG12	1:A:88:LEU:HB3	1.78	0.64
1:A:118:ARG:NH2	1:A:192:GLU:OE2	2.30	0.64
1:B:122:ASN:CG	1:B:230:CYS:SG	2.76	0.64
1:C:556:CYS:SG	1:C:557:ALA:N	2.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:CYS:SG	1:B:557:ALA:N	2.71	0.63
1:C:122:ASN:CG	1:C:230:CYS:SG	2.76	0.63
1:A:122:ASN:CG	1:A:230:CYS:SG	2.76	0.63
1:B:56:ASN:HA	1:B:191:ARG:HH12	1.64	0.63
1:A:556:CYS:SG	1:A:557:ALA:N	2.71	0.63
1:B:80:ASN:C	1:B:109:SER:HB3	2.17	0.63
1:A:74:PHE:O	1:A:75:GLN:NE2	2.31	0.63
1:A:182:PHE:CB	1:B:296:TYR:HB2	2.28	0.63
1:B:74:PHE:O	1:B:75:GLN:NE2	2.31	0.63
1:C:80:ASN:OD1	1:C:235:ALA:HA	1.99	0.63
1:C:115:ASP:OD2	1:C:237:TYR:N	2.32	0.63
1:A:56:ASN:HA	1:A:191:ARG:HH12	1.64	0.63
1:B:115:ASP:OD2	1:B:237:TYR:N	2.32	0.63
1:B:713:LYS:HE2	1:C:534:PHE:CE1	2.34	0.63
1:B:96:TYR:CD1	5:B:1201:NAG:H82	2.34	0.62
1:C:74:PHE:O	1:C:75:GLN:NE2	2.31	0.62
1:A:78:LEU:CD1	1:A:236:SER:O	2.43	0.62
1:B:118:ARG:NH2	1:B:192:GLU:OE2	2.30	0.62
1:A:80:ASN:OD1	1:A:235:ALA:HA	1.99	0.62
1:C:609:SER:O	1:C:613:CYS:HB2	2.00	0.62
1:B:80:ASN:OD1	1:B:235:ALA:HA	1.99	0.62
1:A:115:ASP:OD2	1:A:237:TYR:N	2.32	0.62
1:A:96:TYR:CG	5:A:1201:NAG:C8	2.83	0.61
1:C:88:LEU:HD11	1:C:229:PHE:HB2	1.82	0.61
1:A:631:LYS:CE	1:B:266:GLN:HA	2.31	0.61
1:C:339:LEU:HG	1:C:387:PHE:O	2.00	0.61
1:A:88:LEU:HD11	1:A:229:PHE:HB2	1.82	0.61
1:A:339:LEU:HG	1:A:387:PHE:O	2.00	0.61
1:A:609:SER:O	1:A:613:CYS:HB2	2.00	0.61
1:B:96:TYR:CG	5:B:1201:NAG:C8	2.83	0.61
1:B:339:LEU:HG	1:B:387:PHE:O	2.00	0.61
1:B:609:SER:O	1:B:613:CYS:HB2	2.00	0.61
1:C:56:ASN:HA	1:C:191:ARG:HH12	1.64	0.61
1:C:96:TYR:CG	5:C:1201:NAG:C8	2.83	0.61
1:C:96:TYR:CD1	5:C:1201:NAG:H82	2.34	0.61
1:C:118:ARG:NH2	1:C:192:GLU:OE2	2.30	0.61
1:B:631:LYS:HE2	1:C:266:GLN:HA	1.83	0.61
1:A:182:PHE:HB2	1:B:296:TYR:CD2	2.35	0.60
1:B:713:LYS:HE2	1:C:534:PHE:HE1	1.65	0.60
1:B:96:TYR:CD2	5:B:1201:NAG:C8	2.85	0.60
1:A:821:GLN:O	1:A:824:GLN:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:CD1	1:B:236:SER:O	2.43	0.60
1:A:294:PRO:HB2	1:C:185:ALA:HB2	1.84	0.60
1:C:862:ILE:HD12	1:C:862:ILE:H	1.66	0.60
1:A:862:ILE:HD12	1:A:862:ILE:H	1.66	0.60
1:B:624:LYS:HG3	1:C:72:ARG:NH2	2.17	0.60
1:B:88:LEU:HD11	1:B:229:PHE:HB2	1.82	0.59
1:B:821:GLN:O	1:B:824:GLN:HG2	2.02	0.59
1:C:96:TYR:CD2	5:C:1201:NAG:C8	2.85	0.59
1:A:96:TYR:CD2	5:A:1201:NAG:C8	2.85	0.59
1:A:326:ASN:HB3	5:A:1205:NAG:O5	2.02	0.59
1:B:862:ILE:HD12	1:B:862:ILE:H	1.66	0.59
1:C:529:GLU:HG3	1:C:534:PHE:CE1	2.38	0.59
1:C:821:GLN:O	1:C:824:GLN:HG2	2.02	0.59
1:A:398:MET:O	1:A:414:SER:O	2.21	0.59
1:C:967:CYS:SG	1:C:1018:PHE:HB2	2.42	0.59
1:A:311:GLN:OE1	1:A:311:GLN:N	2.30	0.59
1:A:206:TYR:HE1	1:A:208:TYR:CZ	2.21	0.59
1:A:307:ASP:HA	1:A:354:TYR:HB3	1.85	0.59
1:A:529:GLU:HG3	1:A:534:PHE:CE1	2.38	0.59
1:B:529:GLU:HG3	1:B:534:PHE:CE1	2.37	0.59
1:B:967:CYS:SG	1:B:1018:PHE:HB2	2.42	0.59
1:C:398:MET:O	1:C:414:SER:O	2.21	0.59
1:A:567:ARG:NH2	3:G:1:NAG:O6	2.36	0.58
1:B:115:ASP:OD1	1:B:116:VAL:N	2.37	0.58
1:B:311:GLN:OE1	1:B:311:GLN:N	2.30	0.58
1:A:88:LEU:HD21	1:A:229:PHE:HB2	1.85	0.58
1:B:88:LEU:HD21	1:B:229:PHE:HB2	1.85	0.58
1:B:307:ASP:HA	1:B:354:TYR:HB3	1.85	0.58
1:B:398:MET:O	1:B:414:SER:O	2.21	0.58
1:B:206:TYR:HE1	1:B:208:TYR:CZ	2.21	0.58
1:C:115:ASP:OD1	1:C:116:VAL:N	2.37	0.58
1:A:967:CYS:SG	1:A:1018:PHE:HB2	2.43	0.58
1:C:88:LEU:HD21	1:C:229:PHE:HB2	1.86	0.58
1:B:184:GLY:HA3	1:C:295:VAL:HA	1.85	0.58
1:A:168:CYS:SG	1:A:186:LEU:HD22	2.44	0.58
1:A:631:LYS:HZ1	1:B:266:GLN:HA	1.69	0.58
1:A:54:PHE:HB2	1:A:57:TRP:HB2	1.86	0.57
1:A:115:ASP:OD1	1:A:116:VAL:N	2.37	0.57
1:B:81:CYS:H	1:B:234:LEU:HD21	1.69	0.57
1:C:168:CYS:SG	1:C:186:LEU:HD22	2.44	0.57
1:C:206:TYR:HE1	1:C:208:TYR:CZ	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:THR:HG1	1:A:346:PHE:HB3	1.68	0.57
1:B:168:CYS:SG	1:B:186:LEU:HD22	2.44	0.57
1:B:54:PHE:HB2	1:B:57:TRP:HB2	1.86	0.57
1:A:96:TYR:CG	5:A:1201:NAG:H83	2.40	0.57
1:A:391:ASP:HA	1:A:416:TYR:CG	2.39	0.57
1:B:914:VAL:O	1:B:918:VAL:CB	2.53	0.57
1:C:307:ASP:HA	1:C:354:TYR:HB3	1.85	0.57
1:B:391:ASP:HA	1:B:416:TYR:CG	2.39	0.57
1:C:391:ASP:HA	1:C:416:TYR:CG	2.39	0.57
1:A:81:CYS:H	1:A:234:LEU:HD21	1.69	0.56
1:C:54:PHE:HB2	1:C:57:TRP:HB2	1.86	0.56
1:C:914:VAL:O	1:C:918:VAL:CB	2.53	0.56
1:B:114:SER:HB2	1:B:234:LEU:HD12	1.87	0.56
1:A:914:VAL:O	1:A:918:VAL:CB	2.53	0.56
1:C:82:LEU:H	1:C:105:CYS:HA	1.71	0.56
1:A:391:ASP:N	1:A:391:ASP:OD1	2.39	0.56
1:C:114:SER:HB2	1:C:234:LEU:HD12	1.87	0.56
1:A:82:LEU:H	1:A:105:CYS:HA	1.71	0.56
1:C:81:CYS:H	1:C:234:LEU:HD21	1.69	0.56
1:C:78:LEU:CD1	1:C:236:SER:O	2.43	0.56
1:C:114:SER:OG	1:C:235:ALA:N	2.39	0.56
1:C:953:LEU:HD21	3:O:1:NAG:H3	1.88	0.56
1:B:953:LEU:HD21	3:K:1:NAG:H3	1.88	0.55
1:A:270:ASP:OD1	1:A:270:ASP:N	2.40	0.55
1:A:608:CYS:O	1:A:612:VAL:HG22	2.06	0.55
1:C:79:LEU:HD11	1:C:108:PHE:CG	2.40	0.55
1:C:608:CYS:O	1:C:612:VAL:HG12	2.06	0.55
1:B:82:LEU:H	1:B:105:CYS:HA	1.70	0.55
1:A:114:SER:HB2	1:A:234:LEU:HD12	1.87	0.55
1:A:185:ALA:HB2	1:B:294:PRO:CB	2.36	0.55
1:B:608:CYS:O	1:B:612:VAL:HG22	2.06	0.55
1:B:712:TYR:O	1:B:715:CYS:N	2.29	0.55
1:C:311:GLN:OE1	1:C:311:GLN:N	2.30	0.55
1:B:114:SER:OG	1:B:235:ALA:N	2.39	0.55
1:B:552:SER:HG	1:B:553:PHE:HD2	1.55	0.54
1:A:114:SER:OG	1:A:235:ALA:N	2.39	0.54
1:C:468:LEU:HD23	1:C:468:LEU:H	1.72	0.54
1:A:502:GLN:HB3	1:A:514:MET:HB2	1.90	0.54
1:B:270:ASP:OD1	1:B:270:ASP:N	2.40	0.54
1:A:122:ASN:HD22	5:A:1202:NAG:H83	1.73	0.54
1:B:369:CYS:N	1:B:396:CYS:SG	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:CYS:N	1:A:396:CYS:SG	2.81	0.54
1:B:567:ARG:NH2	3:K:1:NAG:O6	2.41	0.54
1:C:552:SER:HG	1:C:553:PHE:HD2	1.54	0.54
1:C:369:CYS:N	1:C:396:CYS:SG	2.81	0.54
1:C:502:GLN:HB3	1:C:514:MET:HB2	1.90	0.54
1:B:978:GLN:N	1:B:978:GLN:OE1	2.41	0.54
1:B:170:VAL:O	1:B:181:ALA:HB3	2.08	0.54
1:B:502:GLN:HB3	1:B:514:MET:HB2	1.90	0.54
1:B:326:ASN:HB3	5:B:1205:NAG:O5	2.08	0.54
1:C:96:TYR:CG	5:C:1201:NAG:H83	2.43	0.54
1:C:170:VAL:O	1:C:181:ALA:HB3	2.08	0.54
1:A:296:TYR:CD2	1:C:182:PHE:HB2	2.41	0.53
1:B:468:LEU:HD23	1:B:468:LEU:H	1.72	0.53
1:B:613:CYS:HA	1:B:619:CYS:SG	2.48	0.53
1:C:978:GLN:OE1	1:C:978:GLN:N	2.41	0.53
1:B:391:ASP:OD1	1:B:391:ASP:N	2.39	0.53
1:C:270:ASP:N	1:C:270:ASP:OD1	2.40	0.53
1:C:567:ARG:NH2	3:O:1:NAG:O6	2.40	0.53
1:C:613:CYS:HA	1:C:619:CYS:SG	2.48	0.53
1:A:468:LEU:HD23	1:A:468:LEU:H	1.72	0.53
1:A:507:GLN:C	1:A:508:GLN:OE1	2.47	0.53
1:B:588:TRP:HH2	1:B:997:MET:HG2	1.74	0.53
1:C:712:TYR:O	1:C:715:CYS:N	2.29	0.53
1:A:170:VAL:O	1:A:181:ALA:HB3	2.08	0.53
1:A:978:GLN:N	1:A:978:GLN:OE1	2.41	0.53
1:B:354:TYR:OH	1:B:362:ALA:N	2.42	0.53
1:B:507:GLN:C	1:B:508:GLN:OE1	2.47	0.53
1:C:303:VAL:O	1:C:329:LEU:HB2	2.08	0.53
1:C:354:TYR:OH	1:C:362:ALA:N	2.42	0.53
1:C:507:GLN:C	1:C:508:GLN:OE1	2.47	0.53
1:C:633:ILE:HD13	1:C:889:LEU:HD23	1.91	0.53
1:A:303:VAL:O	1:A:329:LEU:HB2	2.08	0.53
1:B:96:TYR:CG	5:B:1201:NAG:H83	2.43	0.53
1:B:256:ASN:OD1	1:B:257:SER:N	2.42	0.53
1:C:391:ASP:OD1	1:C:391:ASP:N	2.39	0.53
1:C:256:ASN:OD1	1:C:257:SER:N	2.42	0.53
1:B:105:CYS:HB3	1:B:109:SER:OG	2.09	0.53
1:B:633:ILE:HD13	1:B:889:LEU:HD23	1.91	0.53
1:C:105:CYS:HB3	1:C:109:SER:OG	2.09	0.53
1:C:326:ASN:HB3	5:C:1205:NAG:O5	2.08	0.53
1:A:208:TYR:CD1	1:B:293:LEU:HD11	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:ASN:HA	1:A:845:ASN:HB2	1.91	0.52
1:A:613:CYS:HA	1:A:619:CYS:SG	2.48	0.52
1:B:590:THR:CG2	1:B:794:LEU:HB2	2.39	0.52
1:A:354:TYR:OH	1:A:362:ALA:N	2.42	0.52
1:A:588:TRP:HH2	1:A:997:MET:HG2	1.73	0.52
1:B:300:THR:HG1	1:B:346:PHE:CB	2.20	0.52
1:B:303:VAL:O	1:B:329:LEU:HB2	2.09	0.52
1:C:78:LEU:HD22	1:C:236:SER:HB2	0.73	0.52
1:C:124:GLU:OE1	1:C:124:GLU:N	2.36	0.52
1:C:311:GLN:OE1	1:C:322:PRO:HB2	2.09	0.52
1:A:68:ASP:CA	1:A:244:VAL:O	2.44	0.52
1:A:88:LEU:HD23	1:A:88:LEU:H	1.75	0.52
1:B:529:GLU:HG3	1:B:534:PHE:HE1	1.75	0.52
1:A:327:ILE:O	1:A:327:ILE:HG13	2.10	0.52
1:B:78:LEU:HD22	1:B:236:SER:HB2	0.73	0.52
1:A:144:TYR:OH	1:A:154:ASP:O	2.27	0.52
1:B:182:PHE:HB2	1:C:296:TYR:HD2	1.75	0.52
1:B:311:GLN:OE1	1:B:322:PRO:HB2	2.09	0.52
1:A:122:ASN:H	1:A:229:PHE:HD1	1.57	0.51
1:A:79:LEU:HD11	1:A:108:PHE:CG	2.40	0.51
1:A:590:THR:CG2	1:A:794:LEU:HB2	2.39	0.51
1:B:122:ASN:H	1:B:229:PHE:HD1	1.57	0.51
1:B:762:THR:N	1:C:582:LEU:HA	2.25	0.51
1:C:773:ILE:HD11	1:C:791:GLN:HG2	1.92	0.51
1:C:842:ASN:HA	1:C:845:ASN:HB2	1.91	0.51
1:A:105:CYS:HB3	1:A:109:SER:OG	2.09	0.51
1:C:327:ILE:HG13	1:C:327:ILE:O	2.10	0.51
1:A:311:GLN:OE1	1:A:322:PRO:HB2	2.09	0.51
1:B:820:SER:OG	1:B:823:LEU:HD23	2.11	0.51
1:B:842:ASN:HA	1:B:845:ASN:HB2	1.91	0.51
1:A:529:GLU:HG3	1:A:534:PHE:HE1	1.75	0.51
1:A:633:ILE:HD13	1:A:889:LEU:HD23	1.91	0.51
1:B:88:LEU:HD23	1:B:88:LEU:H	1.75	0.51
1:C:590:THR:CG2	1:C:794:LEU:HB2	2.39	0.51
1:B:790:ASN:HA	1:B:793:ILE:HG12	1.93	0.51
1:C:88:LEU:H	1:C:88:LEU:HD23	1.75	0.51
1:C:122:ASN:HD22	5:C:1202:NAG:H83	1.76	0.51
1:C:529:GLU:HG3	1:C:534:PHE:HE1	1.75	0.51
1:A:790:ASN:HA	1:A:793:ILE:HG12	1.93	0.51
1:A:97:PHE:O	1:A:113:LEU:HD12	2.11	0.51
1:B:870:ASP:OD1	1:C:372:SER:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLN:HA	1:C:631:LYS:CE	2.40	0.51
1:C:122:ASN:H	1:C:229:PHE:HD1	1.57	0.51
1:A:256:ASN:OD1	1:A:257:SER:N	2.42	0.50
1:A:295:VAL:HA	1:C:184:GLY:HA3	1.92	0.50
1:B:97:PHE:O	1:B:113:LEU:HD12	2.11	0.50
1:A:530:LEU:HD23	1:A:533:PHE:CE1	2.46	0.50
1:A:631:LYS:NZ	1:B:266:GLN:HA	2.25	0.50
1:A:773:ILE:HD11	1:A:791:GLN:HG2	1.92	0.50
1:A:820:SER:OG	1:A:823:LEU:HD23	2.11	0.50
1:B:79:LEU:HD11	1:B:108:PHE:CG	2.40	0.50
1:B:530:LEU:HD23	1:B:533:PHE:CE1	2.46	0.50
1:B:773:ILE:HD11	1:B:791:GLN:HG2	1.92	0.50
1:A:296:TYR:HB2	1:C:182:PHE:HB2	1.94	0.50
1:A:308:PHE:HE2	1:A:318:PHE:CE2	2.30	0.50
1:B:327:ILE:O	1:B:327:ILE:HG13	2.10	0.50
1:C:820:SER:OG	1:C:823:LEU:HD23	2.11	0.50
1:A:762:THR:N	1:B:582:LEU:HA	2.27	0.50
1:B:122:ASN:HD22	5:B:1202:NAG:H83	1.76	0.50
1:C:97:PHE:O	1:C:113:LEU:HD12	2.11	0.50
1:A:624:LYS:HG3	1:B:72:ARG:NH2	2.26	0.50
1:B:821:GLN:CD	1:B:821:GLN:H	2.15	0.50
1:C:530:LEU:HD23	1:C:533:PHE:CE1	2.46	0.50
1:A:383:GLY:N	1:A:420:SER:O	2.33	0.50
1:B:522:TYR:HB2	1:B:524:PHE:HD2	1.77	0.50
1:A:372:SER:CB	1:C:870:ASP:OD1	2.60	0.49
1:B:308:PHE:HE2	1:B:318:PHE:CE2	2.30	0.49
1:A:821:GLN:H	1:A:821:GLN:CD	2.15	0.49
1:B:78:LEU:HD11	1:B:237:TYR:O	2.12	0.49
1:B:793:ILE:HG13	1:B:794:LEU:N	2.28	0.49
1:C:308:PHE:HE2	1:C:318:PHE:CE2	2.29	0.49
1:C:821:GLN:CD	1:C:821:GLN:H	2.15	0.49
1:A:185:ALA:HB2	1:B:294:PRO:HD2	1.95	0.49
1:A:522:TYR:HB2	1:A:524:PHE:HD2	1.77	0.49
1:B:345:HIS:HB3	1:B:433:GLU:OE1	2.12	0.49
1:C:790:ASN:HA	1:C:793:ILE:HG12	1.93	0.49
1:C:308:PHE:HD1	1:C:324:GLY:HA2	1.78	0.49
1:A:345:HIS:HB3	1:A:433:GLU:OE1	2.12	0.49
1:C:345:HIS:HB3	1:C:433:GLU:OE1	2.12	0.49
1:B:308:PHE:HD1	1:B:324:GLY:HA2	1.78	0.49
1:C:78:LEU:HD11	1:C:237:TYR:O	2.12	0.49
1:C:115:ASP:CG	1:C:236:SER:HA	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD11	1:A:237:TYR:O	2.12	0.48
1:A:246:GLN:HB3	1:B:467:PHE:HE1	1.78	0.48
1:C:588:TRP:HH2	1:C:997:MET:HG2	1.74	0.48
1:A:115:ASP:CG	1:A:236:SER:HA	2.33	0.48
1:A:446:CYS:SG	1:A:497:CYS:HB2	2.53	0.48
1:C:793:ILE:HG13	1:C:794:LEU:N	2.28	0.48
1:A:145:CYS:HA	1:A:168:CYS:HA	1.96	0.48
1:A:308:PHE:HD1	1:A:324:GLY:HA2	1.78	0.48
1:B:85:VAL:HG12	1:B:85:VAL:O	2.13	0.48
1:B:115:ASP:CG	1:B:236:SER:HA	2.33	0.48
1:B:766:SER:OG	1:B:767:ILE:N	2.47	0.48
1:C:144:TYR:OH	1:C:154:ASP:O	2.27	0.48
1:C:300:THR:HG1	1:C:346:PHE:HB3	1.75	0.48
1:A:766:SER:OG	1:A:767:ILE:N	2.47	0.48
1:A:971:ARG:O	1:A:1014:CYS:HB2	2.14	0.48
1:B:446:CYS:SG	1:B:497:CYS:HB2	2.53	0.48
1:C:85:VAL:HG12	1:C:85:VAL:O	2.13	0.48
1:C:446:CYS:SG	1:C:497:CYS:HB2	2.53	0.48
1:C:522:TYR:HB2	1:C:524:PHE:HD2	1.77	0.48
1:A:712:TYR:O	1:A:715:CYS:N	2.29	0.48
1:A:793:ILE:HG13	1:A:794:LEU:N	2.28	0.48
1:A:856:GLN:HB3	1:A:880:ARG:HD3	1.96	0.48
1:B:201:PHE:O	1:B:207:ARG:HG2	2.14	0.48
1:B:202:TYR:CE2	1:B:207:ARG:HB2	2.49	0.48
1:B:390:LYS:O	1:B:416:TYR:HB2	2.14	0.48
1:C:96:TYR:CG	5:C:1201:NAG:H82	2.48	0.48
1:C:201:PHE:O	1:C:207:ARG:HG2	2.14	0.48
1:C:766:SER:OG	1:C:767:ILE:N	2.47	0.48
1:A:85:VAL:HG12	1:A:85:VAL:O	2.13	0.48
1:A:96:TYR:CD1	5:A:1201:NAG:C8	2.97	0.48
1:A:202:TYR:CE2	1:A:207:ARG:HB2	2.49	0.48
1:A:302:ILE:HG12	1:A:302:ILE:O	2.14	0.48
1:B:145:CYS:HA	1:B:168:CYS:HA	1.96	0.48
1:B:856:GLN:HB3	1:B:880:ARG:HD3	1.96	0.48
1:A:78:LEU:HD22	1:A:236:SER:HB2	0.73	0.48
1:A:201:PHE:O	1:A:207:ARG:HG2	2.14	0.48
1:B:302:ILE:HG12	1:B:302:ILE:O	2.14	0.48
1:B:144:TYR:OH	1:B:154:ASP:O	2.27	0.47
1:B:68:ASP:CA	1:B:244:VAL:O	2.44	0.47
1:B:741:ASP:OD1	1:B:741:ASP:N	2.43	0.47
1:C:202:TYR:CE2	1:C:207:ARG:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:TYR:CG	5:A:1201:NAG:H82	2.49	0.47
1:A:390:LYS:O	1:A:416:TYR:HB2	2.14	0.47
1:B:971:ARG:O	1:B:1014:CYS:HB2	2.14	0.47
1:C:322:PRO:C	1:C:324:GLY:H	2.18	0.47
1:C:390:LYS:O	1:C:416:TYR:HB2	2.13	0.47
1:C:741:ASP:N	1:C:741:ASP:OD1	2.43	0.47
1:C:971:ARG:O	1:C:1014:CYS:HB2	2.14	0.47
1:C:115:ASP:HA	1:C:197:ARG:HH12	1.80	0.47
1:B:322:PRO:C	1:B:324:GLY:H	2.18	0.47
1:C:68:ASP:CA	1:C:244:VAL:O	2.44	0.47
1:C:302:ILE:O	1:C:302:ILE:HG12	2.14	0.47
1:C:331:ASN:HB3	1:C:339:LEU:HD22	1.96	0.47
1:C:618:ARG:HB2	1:C:866:TYR:CE2	2.49	0.47
1:A:518:ASN:HD22	5:A:1206:NAG:C7	2.28	0.47
1:A:618:ARG:HB2	1:A:866:TYR:CE2	2.49	0.47
1:B:618:ARG:HB2	1:B:866:TYR:CE2	2.49	0.47
1:C:145:CYS:HA	1:C:168:CYS:HA	1.96	0.47
1:B:115:ASP:HA	1:B:197:ARG:HH12	1.80	0.47
1:B:383:GLY:N	1:B:420:SER:O	2.33	0.47
1:C:540:THR:O	1:C:560:SER:OG	2.33	0.47
1:C:969:ASP:HB3	1:C:1022:SER:HA	1.97	0.47
1:A:1020:ASN:HB3	5:A:1216:NAG:N2	2.29	0.47
1:B:230:CYS:CB	5:B:1202:NAG:H83	2.42	0.47
1:C:575:SER:OG	1:C:995:ARG:CD	2.59	0.47
1:A:331:ASN:HB3	1:A:339:LEU:HD22	1.96	0.46
1:A:552:SER:HG	1:A:553:PHE:HD2	1.59	0.46
1:C:934:ILE:HD11	1:C:952:LEU:HD11	1.97	0.46
1:B:331:ASN:HB3	1:B:339:LEU:HD22	1.96	0.46
1:B:969:ASP:HB3	1:B:1022:SER:HA	1.97	0.46
1:C:297:HIS:HB2	1:C:434:GLY:N	2.30	0.46
1:C:617:VAL:O	1:C:621:GLU:HG2	2.16	0.46
1:C:856:GLN:HB3	1:C:880:ARG:HD3	1.96	0.46
1:A:297:HIS:HB2	1:A:434:GLY:N	2.31	0.46
1:C:333:ASN:OD1	1:C:334:GLU:N	2.49	0.46
1:B:297:HIS:HB2	1:B:434:GLY:N	2.30	0.46
1:B:984:TYR:CE2	1:B:986:GLU:HB2	2.51	0.46
1:A:115:ASP:HA	1:A:197:ARG:HH12	1.80	0.46
1:B:983:LEU:HD12	1:B:984:TYR:H	1.81	0.46
1:C:385:VAL:O	1:C:418:SER:O	2.34	0.46
1:A:461:ARG:NH1	1:C:716:THR:O	2.48	0.46
1:A:543:CYS:HA	1:A:562:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:LYS:CE	1:C:266:GLN:HA	2.45	0.46
1:C:991:ARG:HD3	1:C:991:ARG:HA	1.67	0.46
1:A:332:PHE:HA	1:A:336:LYS:HZ2	1.81	0.46
1:A:385:VAL:O	1:A:418:SER:O	2.34	0.46
1:B:96:TYR:CG	1:B:216:ALA:CB	2.95	0.46
1:A:322:PRO:C	1:A:324:GLY:H	2.18	0.46
1:A:333:ASN:OD1	1:A:334:GLU:N	2.49	0.46
1:B:124:GLU:OE1	1:B:124:GLU:N	2.36	0.46
1:C:983:LEU:HD12	1:C:984:TYR:H	1.80	0.46
1:A:969:ASP:HB3	1:A:1022:SER:HA	1.96	0.46
1:A:984:TYR:CE2	1:A:986:GLU:HB2	2.51	0.46
1:B:338:PRO:HG3	1:B:392:ILE:HD11	1.98	0.46
1:B:543:CYS:HA	1:B:562:ILE:HD11	1.97	0.46
1:B:617:VAL:O	1:B:621:GLU:HG2	2.16	0.46
1:A:789:GLU:O	1:A:793:ILE:HG12	2.16	0.46
1:B:96:TYR:CG	5:B:1201:NAG:H82	2.48	0.46
1:A:305:TYR:CE1	1:A:351:VAL:HG11	2.51	0.45
1:A:934:ILE:HD11	1:A:952:LEU:HD11	1.97	0.45
1:A:983:LEU:HD12	1:A:984:TYR:H	1.81	0.45
1:A:991:ARG:HA	1:A:991:ARG:HD3	1.67	0.45
1:B:106:LYS:HG2	1:B:106:LYS:O	2.16	0.45
1:A:540:THR:O	1:A:560:SER:OG	2.33	0.45
1:A:617:VAL:O	1:A:621:GLU:HG2	2.16	0.45
1:A:289:SER:OG	1:A:441:VAL:HA	2.16	0.45
1:B:305:TYR:CE1	1:B:351:VAL:HG21	2.51	0.45
1:B:333:ASN:OD1	1:B:334:GLU:N	2.49	0.45
1:B:692:ILE:H	1:B:692:ILE:HG12	1.52	0.45
1:B:789:GLU:O	1:B:793:ILE:HG12	2.16	0.45
1:B:995:ARG:CZ	1:B:996:ILE:HD11	2.47	0.45
1:C:106:LYS:O	1:C:106:LYS:HG2	2.16	0.45
1:C:789:GLU:O	1:C:793:ILE:HG12	2.16	0.45
1:C:984:TYR:CE2	1:C:986:GLU:HB2	2.51	0.45
1:A:55:ASN:OD1	1:A:56:ASN:N	2.50	0.45
1:A:124:GLU:OE1	1:A:124:GLU:N	2.36	0.45
1:B:124:GLU:H	1:B:124:GLU:CD	2.18	0.45
1:B:188:LYS:HD2	1:B:188:LYS:C	2.37	0.45
1:B:385:VAL:O	1:B:418:SER:O	2.34	0.45
1:C:88:LEU:O	1:C:89:ARG:HD3	2.17	0.45
1:C:305:TYR:CE1	1:C:351:VAL:HG11	2.51	0.45
1:C:338:PRO:HG3	1:C:392:ILE:HD11	1.98	0.45
1:A:741:ASP:N	1:A:741:ASP:OD1	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:SER:OG	1:B:995:ARG:CD	2.59	0.45
1:B:937:LEU:HB2	1:B:948:LEU:HB2	1.99	0.45
1:C:526:ASN:OD1	1:C:527:VAL:N	2.50	0.45
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.79	0.45
1:B:88:LEU:O	1:B:89:ARG:HD3	2.17	0.45
1:C:289:SER:OG	1:C:441:VAL:HA	2.16	0.45
1:A:185:ALA:HB2	1:B:294:PRO:CD	2.47	0.45
1:A:338:PRO:HG3	1:A:392:ILE:HD11	1.98	0.45
1:A:995:ARG:CZ	1:A:996:ILE:HD11	2.47	0.45
1:B:55:ASN:OD1	1:B:56:ASN:N	2.50	0.45
1:B:526:ASN:OD1	1:B:527:VAL:N	2.50	0.45
1:B:934:ILE:HD11	1:B:952:LEU:HD11	1.97	0.45
1:C:78:LEU:HB2	1:C:236:SER:N	2.28	0.45
1:A:670:TYR:HD2	1:A:798:PHE:CD2	2.35	0.45
1:B:148:ASN:HB3	1:B:153:GLY:HA2	1.99	0.45
1:B:336:LYS:HD2	1:B:336:LYS:HA	1.78	0.45
1:A:106:LYS:O	1:A:106:LYS:HG2	2.16	0.45
1:A:188:LYS:C	1:A:188:LYS:HD2	2.37	0.45
1:A:460:ILE:HD12	1:A:460:ILE:N	2.32	0.45
1:B:460:ILE:N	1:B:460:ILE:HD12	2.32	0.45
1:B:582:LEU:O	1:B:960:VAL:N	2.50	0.45
1:C:78:LEU:HB3	1:C:80:ASN:ND2	2.32	0.45
1:C:188:LYS:HD2	1:C:188:LYS:C	2.37	0.45
1:C:543:CYS:HA	1:C:562:ILE:HD11	1.98	0.45
1:C:582:LEU:O	1:C:960:VAL:N	2.50	0.45
1:A:351:VAL:HG12	1:A:352:ALA:H	1.82	0.45
1:B:289:SER:OG	1:B:441:VAL:HA	2.16	0.45
1:A:124:GLU:H	1:A:124:GLU:CD	2.18	0.44
1:A:273:ASP:HB3	1:A:506:TYR:HA	1.99	0.44
1:A:364:ILE:HD12	1:A:364:ILE:HA	1.73	0.44
1:B:230:CYS:SG	5:B:1202:NAG:C7	3.03	0.44
1:B:273:ASP:HB3	1:B:506:TYR:HA	1.99	0.44
1:B:351:VAL:HG22	1:B:352:ALA:H	1.82	0.44
1:B:540:THR:O	1:B:560:SER:OG	2.33	0.44
1:A:410:TYR:CE1	1:B:338:PRO:HD2	2.52	0.44
1:A:762:THR:H	1:B:582:LEU:HA	1.83	0.44
1:A:899:LYS:O	1:A:902:GLU:HG3	2.17	0.44
1:A:526:ASN:OD1	1:A:527:VAL:N	2.50	0.44
1:B:300:THR:HG1	1:B:346:PHE:HB3	1.77	0.44
1:B:890:ASN:HA	1:B:893:VAL:HG12	2.00	0.44
1:C:124:GLU:H	1:C:124:GLU:CD	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:692:ILE:H	1:C:692:ILE:HG12	1.52	0.44
1:C:995:ARG:CZ	1:C:996:ILE:HD11	2.47	0.44
1:A:78:LEU:HB3	1:A:80:ASN:ND2	2.32	0.44
1:A:88:LEU:O	1:A:89:ARG:HD3	2.17	0.44
1:B:78:LEU:HB3	1:B:80:ASN:ND2	2.32	0.44
1:C:148:ASN:HB3	1:C:153:GLY:HA2	1.99	0.44
1:C:273:ASP:HB3	1:C:506:TYR:HA	1.99	0.44
1:A:321:TYR:HB2	1:A:410:TYR:CE2	2.53	0.44
1:C:321:TYR:HB2	1:C:410:TYR:CE2	2.53	0.44
1:C:383:GLY:N	1:C:420:SER:O	2.33	0.44
1:C:460:ILE:HD12	1:C:460:ILE:N	2.32	0.44
1:A:148:ASN:HB3	1:A:153:GLY:HA2	1.99	0.44
1:C:670:TYR:HD2	1:C:798:PHE:CD2	2.35	0.44
1:C:674:SER:O	1:C:690:SER:HB3	2.18	0.44
1:A:185:ALA:CB	1:B:294:PRO:HB2	2.45	0.44
1:A:969:ASP:OD1	1:A:970:GLY:N	2.50	0.44
1:A:575:SER:OG	1:A:995:ARG:CD	2.59	0.44
1:A:937:LEU:HB2	1:A:948:LEU:HB2	1.99	0.44
1:B:78:LEU:HB2	1:B:236:SER:N	2.28	0.44
1:C:55:ASN:OD1	1:C:56:ASN:N	2.50	0.44
1:A:890:ASN:HA	1:A:893:VAL:HG12	2.00	0.44
1:B:547:VAL:HG11	1:B:557:ALA:HA	2.00	0.44
1:C:899:LYS:O	1:C:902:GLU:HG3	2.17	0.44
5:C:1201:NAG:O7	5:C:1201:NAG:O3	2.34	0.44
1:B:321:TYR:HB2	1:B:410:TYR:CE2	2.53	0.43
1:B:899:LYS:O	1:B:902:GLU:HG3	2.17	0.43
1:B:264:CYS:SG	1:B:265:ASP:N	2.91	0.43
1:B:382:PHE:HE1	1:B:419:TRP:CG	2.36	0.43
1:C:349:LYS:HE3	1:C:349:LYS:HB2	1.74	0.43
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.92	0.43
1:B:670:TYR:HD2	1:B:798:PHE:CD2	2.35	0.43
1:B:965:GLY:C	1:B:1018:PHE:HB3	2.39	0.43
1:C:969:ASP:OD1	1:C:970:GLY:N	2.50	0.43
1:A:582:LEU:O	1:A:960:VAL:N	2.50	0.43
1:B:96:TYR:CD2	1:B:215:GLU:HG2	2.54	0.43
1:B:802:MET:HA	1:B:805:ILE:HG12	2.01	0.43
1:C:322:PRO:C	1:C:324:GLY:N	2.72	0.43
1:C:382:PHE:HE1	1:C:419:TRP:CG	2.36	0.43
1:C:697:PHE:HE1	1:C:942:PRO:HG3	1.84	0.43
1:C:890:ASN:HA	1:C:893:VAL:HG12	2.00	0.43
1:C:937:LEU:HB2	1:C:948:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:TYR:CD2	1:A:215:GLU:HG2	2.54	0.43
1:A:264:CYS:SG	1:A:265:ASP:N	2.91	0.43
1:A:310:PRO:CB	1:A:322:PRO:HG2	2.48	0.43
1:A:382:PHE:HE1	1:A:419:TRP:CG	2.36	0.43
1:B:185:ALA:N	1:C:294:PRO:O	2.42	0.43
1:B:234:LEU:HD23	1:B:234:LEU:H	1.83	0.43
1:B:697:PHE:HE1	1:B:942:PRO:HG3	1.84	0.43
1:C:965:GLY:C	1:C:1018:PHE:HB3	2.39	0.43
1:C:802:MET:HA	1:C:805:ILE:HG12	2.01	0.43
1:A:96:TYR:CG	1:A:216:ALA:CB	2.95	0.43
1:A:674:SER:O	1:A:690:SER:HB3	2.18	0.43
1:B:310:PRO:CB	1:B:322:PRO:HG2	2.48	0.43
1:B:969:ASP:OD1	1:B:970:GLY:N	2.50	0.43
1:C:96:TYR:CD2	1:C:215:GLU:HG2	2.54	0.43
1:C:206:TYR:HE1	1:C:208:TYR:CE2	2.37	0.43
1:C:310:PRO:CB	1:C:322:PRO:HG2	2.48	0.43
1:C:351:VAL:HG12	1:C:352:ALA:H	1.82	0.43
1:A:697:PHE:HE1	1:A:942:PRO:HG3	1.84	0.43
1:B:116:VAL:HG22	1:B:196:SER:CB	2.49	0.43
1:C:121:LEU:HD12	1:C:229:PHE:CE1	2.54	0.43
1:C:264:CYS:SG	1:C:265:ASP:N	2.91	0.43
1:A:182:PHE:CD1	1:B:296:TYR:N	2.87	0.43
1:A:208:TYR:CE1	1:B:293:LEU:HD11	2.54	0.43
1:A:289:SER:O	1:A:449:TYR:HA	2.19	0.43
1:A:547:VAL:HG11	1:A:557:ALA:HA	2.00	0.43
1:C:116:VAL:HG12	1:C:196:SER:CB	2.49	0.43
1:C:299:HIS:HD2	1:C:433:GLU:HB2	1.84	0.43
1:A:299:HIS:HD2	1:A:433:GLU:HB2	1.84	0.43
1:B:299:HIS:HD2	1:B:433:GLU:HB2	1.84	0.43
1:C:289:SER:O	1:C:449:TYR:HA	2.19	0.43
1:A:116:VAL:HG22	1:A:196:SER:CB	2.49	0.42
1:A:802:MET:HA	1:A:805:ILE:HG12	2.01	0.42
1:A:965:GLY:C	1:A:1018:PHE:HB3	2.39	0.42
1:B:121:LEU:HD12	1:B:229:PHE:CE1	2.54	0.42
1:B:674:SER:O	1:B:690:SER:HB3	2.18	0.42
1:C:299:HIS:HA	1:C:433:GLU:OE1	2.19	0.42
1:C:547:VAL:HG21	1:C:557:ALA:HA	2.00	0.42
1:A:234:LEU:H	1:A:234:LEU:HD23	1.83	0.42
1:B:526:ASN:O	1:B:536:ALA:HA	2.20	0.42
1:A:625:GLN:HG3	1:A:626:TYR:CD1	2.54	0.42
1:B:289:SER:O	1:B:449:TYR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HB2	1:A:236:SER:N	2.28	0.42
1:A:121:LEU:HD12	1:A:229:PHE:CE1	2.54	0.42
1:A:230:CYS:SG	5:A:1202:NAG:C7	3.05	0.42
1:B:122:ASN:HB2	1:B:230:CYS:HG	1.81	0.42
1:B:206:TYR:HE1	1:B:208:TYR:CE2	2.37	0.42
1:B:762:THR:CB	1:C:581:ASN:HB3	2.48	0.42
1:B:967:CYS:HB3	1:B:1014:CYS:SG	2.60	0.42
1:B:1024:SER:OG	1:B:1025:GLU:N	2.53	0.42
1:C:230:CYS:CB	5:C:1202:NAG:H83	2.43	0.42
1:A:206:TYR:HE1	1:A:208:TYR:CE2	2.37	0.42
1:A:322:PRO:C	1:A:324:GLY:N	2.72	0.42
1:A:372:SER:HB2	1:C:870:ASP:OD1	2.18	0.42
1:A:1024:SER:OG	1:A:1025:GLU:N	2.53	0.42
1:B:299:HIS:HA	1:B:433:GLU:OE1	2.19	0.42
1:B:322:PRO:C	1:B:324:GLY:N	2.72	0.42
1:C:1024:SER:OG	1:C:1025:GLU:N	2.53	0.42
1:A:299:HIS:HA	1:A:433:GLU:OE1	2.19	0.42
1:A:526:ASN:O	1:A:536:ALA:HA	2.20	0.42
1:B:96:TYR:CZ	1:B:216:ALA:HB2	2.54	0.42
1:B:297:HIS:HB3	1:B:433:GLU:HB3	2.02	0.42
1:C:297:HIS:HB3	1:C:433:GLU:HB3	2.02	0.42
1:C:297:HIS:HB3	1:C:433:GLU:HG2	2.01	0.42
1:A:582:LEU:HA	1:C:762:THR:N	2.35	0.42
1:C:234:LEU:H	1:C:234:LEU:HD23	1.83	0.42
1:C:297:HIS:CD2	1:C:345:HIS:CE1	3.08	0.42
1:A:195:ILE:HD12	1:A:195:ILE:HA	1.93	0.42
1:A:307:ASP:OD1	1:A:309:LYS:HB2	2.20	0.42
1:B:60:LEU:HD23	1:B:205:GLY:HA2	2.01	0.42
1:B:312:SER:OG	1:B:313:GLY:N	2.53	0.42
1:B:865:ILE:HD13	1:B:865:ILE:HA	1.92	0.42
1:C:60:LEU:HD23	1:C:205:GLY:HA2	2.01	0.42
1:C:364:ILE:HD12	1:C:364:ILE:HA	1.73	0.42
1:C:625:GLN:HG3	1:C:626:TYR:CD1	2.54	0.42
1:C:748:TYR:CE2	1:C:752:LEU:HD11	2.55	0.42
1:A:297:HIS:CD2	1:A:345:HIS:CE1	3.08	0.42
1:A:312:SER:OG	1:A:313:GLY:N	2.53	0.42
1:A:967:CYS:HB3	1:A:1014:CYS:SG	2.60	0.42
1:B:297:HIS:HB3	1:B:433:GLU:HG2	2.01	0.42
1:B:518:ASN:HB2	1:B:534:PHE:CE2	2.55	0.42
1:C:967:CYS:HB3	1:C:1014:CYS:SG	2.60	0.42
1:B:85:VAL:CG1	1:B:88:LEU:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:HD12	1:B:195:ILE:HA	1.93	0.42
1:C:518:ASN:HB2	1:C:534:PHE:CE2	2.55	0.42
1:A:297:HIS:HB3	1:A:433:GLU:HB3	2.02	0.41
1:B:96:TYR:CD1	1:B:216:ALA:HB2	2.55	0.41
1:B:297:HIS:NE2	1:B:345:HIS:HE1	2.18	0.41
1:B:307:ASP:OD1	1:B:309:LYS:HB2	2.20	0.41
1:B:349:LYS:HE3	1:B:349:LYS:HB2	1.74	0.41
1:B:625:GLN:HG3	1:B:626:TYR:CD1	2.54	0.41
1:C:295:VAL:O	1:C:297:HIS:HD2	2.03	0.41
1:A:299:HIS:CD2	1:A:433:GLU:HB2	2.56	0.41
1:B:81:CYS:HB2	1:B:234:LEU:CD2	2.51	0.41
1:C:297:HIS:NE2	1:C:345:HIS:HE1	2.18	0.41
1:A:295:VAL:O	1:A:297:HIS:HD2	2.03	0.41
1:A:480:LEU:H	1:A:480:LEU:HD23	1.85	0.41
1:B:96:TYR:CD1	5:B:1201:NAG:C8	3.01	0.41
1:B:141:VAL:HA	1:B:172:THR:HA	2.02	0.41
1:B:480:LEU:H	1:B:480:LEU:HD23	1.85	0.41
1:B:748:TYR:CE2	1:B:752:LEU:HD11	2.55	0.41
1:C:57:TRP:CZ3	1:C:118:ARG:NE	2.88	0.41
1:C:269:PHE:CD1	1:C:269:PHE:N	2.88	0.41
1:A:297:HIS:HB3	1:A:433:GLU:HG2	2.01	0.41
1:A:748:TYR:CE2	1:A:752:LEU:HD11	2.55	0.41
1:A:778:ASN:HA	1:A:781:ALA:O	2.21	0.41
5:A:1201:NAG:O7	5:A:1201:NAG:O3	2.34	0.41
1:C:480:LEU:HD23	1:C:480:LEU:H	1.85	0.41
1:C:613:CYS:SG	1:C:620:VAL:HA	2.60	0.41
1:A:60:LEU:HD23	1:A:205:GLY:HA2	2.01	0.41
1:A:297:HIS:NE2	1:A:345:HIS:HE1	2.18	0.41
1:C:526:ASN:O	1:C:536:ALA:HA	2.19	0.41
1:C:778:ASN:HA	1:C:781:ALA:O	2.21	0.41
1:B:57:TRP:CZ3	1:B:118:ARG:NE	2.88	0.41
1:B:295:VAL:O	1:B:297:HIS:HD2	2.03	0.41
1:B:572:ASP:OD1	1:B:572:ASP:N	2.53	0.41
1:C:48:ILE:HA	1:C:49:PRO:HD3	1.92	0.41
1:C:312:SER:OG	1:C:313:GLY:N	2.53	0.41
1:A:141:VAL:HA	1:A:172:THR:HA	2.02	0.41
1:A:518:ASN:HB2	1:A:534:PHE:CE2	2.55	0.41
1:B:147:ASN:HB3	1:B:154:ASP:OD2	2.21	0.41
1:B:879:ASP:O	1:B:882:ILE:HG12	2.21	0.41
1:C:299:HIS:CD2	1:C:433:GLU:HB2	2.56	0.41
1:C:711:ASP:OD1	1:C:711:ASP:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:CYS:SG	1:A:620:VAL:HA	2.60	0.41
1:B:269:PHE:CD1	1:B:269:PHE:N	2.88	0.41
1:B:403:ASN:HA	1:B:408:LYS:O	2.20	0.41
1:C:96:TYR:CD1	5:C:1201:NAG:C8	3.01	0.41
1:A:81:CYS:HB2	1:A:234:LEU:CD2	2.50	0.41
1:A:96:TYR:CD1	1:A:216:ALA:HB2	2.55	0.41
1:A:208:TYR:HD1	1:B:293:LEU:HD11	1.85	0.41
1:A:403:ASN:HA	1:A:408:LYS:O	2.20	0.41
1:A:998:PHE:O	1:A:998:PHE:CD2	2.74	0.41
1:B:230:CYS:CB	5:B:1202:NAG:C8	2.99	0.41
1:B:297:HIS:CD2	1:B:345:HIS:CE1	3.08	0.41
1:B:711:ASP:O	1:B:711:ASP:OD1	2.39	0.41
1:C:81:CYS:HB2	1:C:234:LEU:CD2	2.50	0.41
1:C:96:TYR:CG	1:C:216:ALA:CB	2.95	0.41
1:C:147:ASN:HB3	1:C:154:ASP:OD2	2.21	0.41
1:C:230:CYS:SG	5:C:1202:NAG:C7	3.03	0.41
1:C:403:ASN:HA	1:C:408:LYS:O	2.20	0.41
1:C:548:LEU:HB3	1:C:555:VAL:CG2	2.51	0.41
1:B:81:CYS:HB2	1:B:234:LEU:HD21	2.03	0.41
1:C:72:ARG:HA	1:C:241:LEU:HA	2.03	0.41
1:C:85:VAL:CG1	1:C:88:LEU:HB3	2.48	0.41
1:A:185:ALA:N	1:B:294:PRO:O	2.36	0.40
1:A:269:PHE:CD1	1:A:269:PHE:N	2.88	0.40
1:A:349:LYS:HE3	1:A:349:LYS:HB2	1.74	0.40
1:A:1022:SER:OG	1:A:1023:ARG:N	2.54	0.40
1:B:548:LEU:HB3	1:B:555:VAL:CG2	2.51	0.40
1:A:711:ASP:O	1:A:711:ASP:OD1	2.39	0.40
1:B:613:CYS:SG	1:B:620:VAL:HA	2.60	0.40
1:C:81:CYS:HB2	1:C:234:LEU:HD21	2.03	0.40
1:C:307:ASP:OD1	1:C:309:LYS:HB2	2.20	0.40
1:C:1022:SER:OG	1:C:1023:ARG:N	2.54	0.40
1:A:271:VAL:H	1:A:271:VAL:HG12	1.62	0.40
1:A:548:LEU:HB3	1:A:555:VAL:CG1	2.51	0.40
1:B:260:ASN:OD1	1:B:263:ARG:NH1	2.53	0.40
1:B:299:HIS:CD2	1:B:433:GLU:HB2	2.56	0.40
1:B:778:ASN:HA	1:B:781:ALA:O	2.21	0.40
1:C:230:CYS:CB	5:C:1202:NAG:C8	2.99	0.40
1:A:81:CYS:HB2	1:A:234:LEU:HD21	2.03	0.40
1:A:96:TYR:CZ	1:A:216:ALA:HB2	2.54	0.40
1:A:182:PHE:HE2	1:B:298:LYS:HD2	1.86	0.40
1:B:691:ALA:C	1:B:693:GLU:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:998:PHE:O	1:B:998:PHE:CD2	2.74	0.40
1:A:410:TYR:HE1	1:B:338:PRO:HD2	1.85	0.40
1:B:862:ILE:HD12	1:B:862:ILE:N	2.36	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	951/1116 (85%)	893 (94%)	53 (6%)	5 (0%)	25	59
1	B	951/1116 (85%)	893 (94%)	53 (6%)	5 (0%)	25	59
1	C	951/1116 (85%)	893 (94%)	53 (6%)	5 (0%)	25	59
All	All	2853/3348 (85%)	2679 (94%)	159 (6%)	15 (0%)	27	59

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	VAL
1	A	331	ASN
1	A	351	VAL
1	B	325	VAL
1	B	331	ASN
1	B	351	VAL
1	C	325	VAL
1	C	331	ASN
1	C	351	VAL
1	A	399	PRO
1	B	399	PRO
1	B	667	PHE
1	C	399	PRO
1	A	667	PHE

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Mol	Chain	Res	Type
1	C	667	PHE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	731/969 (75%)	687 (94%)	44 (6%)	16	46
1	B	721/969 (74%)	682 (95%)	39 (5%)	18	50
1	C	723/969 (75%)	687 (95%)	36 (5%)	20	52
All	All	2175/2907 (75%)	2056 (94%)	119 (6%)	20	49

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	81	CYS
1	A	88	LEU
1	A	96	TYR
1	A	111	ASP
1	A	117	ILE
1	A	141	VAL
1	A	151	VAL
1	A	183	VAL
1	A	188	LYS
1	A	190	VAL
1	A	194	VAL
1	A	203	ILE
1	A	221	VAL
1	A	228	ASP
1	A	264	CYS
1	A	270	ASP
1	A	271	VAL
1	A	302	ILE
1	A	351	VAL
1	A	353	VAL

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Mol	Chain	Res	Type
1	A	363	SER
1	A	364	ILE
1	A	369	CYS
1	A	382	PHE
1	A	392	ILE
1	A	400	ILE
1	A	401	VAL
1	A	403	ASN
1	A	432	VAL
1	A	547	VAL
1	A	555	VAL
1	A	573	SER
1	A	586	SER
1	A	630	CYS
1	A	672	LEU
1	A	692	ILE
1	A	724	LEU
1	A	770	SER
1	A	779	TYR
1	A	780	VAL
1	A	860	SER
1	A	928	CYS
1	A	953	LEU
1	B	79	LEU
1	B	81	CYS
1	B	88	LEU
1	B	95	VAL
1	B	96	TYR
1	B	111	ASP
1	B	117	ILE
1	B	183	VAL
1	B	188	LYS
1	B	190	VAL
1	B	194	VAL
1	B	203	ILE
1	B	221	VAL
1	B	228	ASP
1	B	264	CYS
1	B	270	ASP
1	B	302	ILE
1	B	353	VAL
1	B	363	SER

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Mol	Chain	Res	Type
1	B	364	ILE
1	B	369	CYS
1	B	382	PHE
1	B	392	ILE
1	B	400	ILE
1	B	403	ASN
1	B	441	VAL
1	B	547	VAL
1	B	573	SER
1	B	586	SER
1	B	630	CYS
1	B	672	LEU
1	B	692	ILE
1	B	724	LEU
1	B	770	SER
1	B	779	TYR
1	B	780	VAL
1	B	860	SER
1	B	928	CYS
1	B	953	LEU
1	C	79	LEU
1	C	81	CYS
1	C	88	LEU
1	C	96	TYR
1	C	111	ASP
1	C	117	ILE
1	C	141	VAL
1	C	183	VAL
1	C	188	LYS
1	C	203	ILE
1	C	228	ASP
1	C	264	CYS
1	C	270	ASP
1	C	271	VAL
1	C	302	ILE
1	C	351	VAL
1	C	353	VAL
1	C	363	SER
1	C	364	ILE
1	C	369	CYS
1	C	382	PHE
1	C	392	ILE

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Mol	Chain	Res	Type
1	C	400	ILE
1	C	403	ASN
1	C	428	VAL
1	C	573	SER
1	C	586	SER
1	C	630	CYS
1	C	672	LEU
1	C	692	ILE
1	C	724	LEU
1	C	770	SER
1	C	779	TYR
1	C	860	SER
1	C	928	CYS
1	C	953	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	345	HIS
1	A	850	GLN
1	A	890	ASN
1	A	933	HIS
1	B	75	GLN
1	B	266	GLN
1	B	345	HIS
1	B	850	GLN
1	B	933	HIS
1	C	75	GLN
1	C	345	HIS
1	C	839	GLN
1	C	890	ASN
1	C	933	HIS

### 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 ⓘ

45 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	0.40	0	17,19,21	1.08	2 (11%)
2	NAG	D	2	2	14,14,15	0.30	0	17,19,21	0.78	0
2	BMA	D	3	2	11,11,12	0.36	0	15,15,17	1.59	4 (26%)
2	MAN	D	4	2	11,11,12	0.20	0	15,15,17	0.94	1 (6%)
2	MAN	D	5	2	11,11,12	0.20	0	15,15,17	0.67	0
2	MAN	D	6	2	11,11,12	0.18	0	15,15,17	1.15	1 (6%)
2	MAN	D	7	2	11,11,12	0.22	0	15,15,17	1.08	1 (6%)
3	NAG	E	1	3,1	14,14,15	0.63	0	17,19,21	0.76	0
3	NAG	E	2	3	14,14,15	0.60	0	17,19,21	0.38	0
3	BMA	E	3	3	11,11,12	0.50	0	15,15,17	0.97	1 (6%)
4	NAG	F	1	4,1	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	F	2	4	14,14,15	0.23	0	17,19,21	0.58	0
3	NAG	G	1	3,1	14,14,15	0.65	0	17,19,21	0.69	1 (5%)
3	NAG	G	2	3	14,14,15	0.51	0	17,19,21	0.38	0
3	BMA	G	3	3	11,11,12	0.52	0	15,15,17	0.97	1 (6%)
2	NAG	H	1	2,1	14,14,15	0.41	0	17,19,21	1.08	1 (5%)
2	NAG	H	2	2	14,14,15	0.32	0	17,19,21	0.79	0
2	BMA	H	3	2	11,11,12	0.37	0	15,15,17	1.59	4 (26%)
2	MAN	H	4	2	11,11,12	0.19	0	15,15,17	0.94	1 (6%)
2	MAN	H	5	2	11,11,12	0.19	0	15,15,17	0.68	0
2	MAN	H	6	2	11,11,12	0.19	0	15,15,17	1.16	1 (6%)
2	MAN	H	7	2	11,11,12	0.22	0	15,15,17	1.08	1 (6%)
3	NAG	I	1	3,1	14,14,15	0.61	0	17,19,21	0.76	0
3	NAG	I	2	3	14,14,15	0.60	0	17,19,21	0.38	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	I	3	3	11,11,12	0.51	0	15,15,17	0.97	1 (6%)
4	NAG	J	1	4,1	14,14,15	0.30	0	17,19,21	0.47	0
4	NAG	J	2	4	14,14,15	0.22	0	17,19,21	0.59	0
3	NAG	K	1	3,1	14,14,15	0.65	0	17,19,21	0.70	1 (5%)
3	NAG	K	2	3	14,14,15	0.53	0	17,19,21	0.39	0
3	BMA	K	3	3	11,11,12	0.51	0	15,15,17	0.97	1 (6%)
2	NAG	L	1	2,1	14,14,15	0.39	0	17,19,21	1.09	2 (11%)
2	NAG	L	2	2	14,14,15	0.31	0	17,19,21	0.77	0
2	BMA	L	3	2	11,11,12	0.37	0	15,15,17	1.59	4 (26%)
2	MAN	L	4	2	11,11,12	0.21	0	15,15,17	0.93	1 (6%)
2	MAN	L	5	2	11,11,12	0.20	0	15,15,17	0.68	0
2	MAN	L	6	2	11,11,12	0.17	0	15,15,17	1.16	1 (6%)
2	MAN	L	7	2	11,11,12	0.22	0	15,15,17	1.06	1 (6%)
3	NAG	M	1	3,1	14,14,15	0.63	0	17,19,21	0.75	0
3	NAG	M	2	3	14,14,15	0.61	0	17,19,21	0.38	0
3	BMA	M	3	3	11,11,12	0.51	0	15,15,17	0.97	1 (6%)
4	NAG	N	1	4,1	14,14,15	0.27	0	17,19,21	0.47	0
4	NAG	N	2	4	14,14,15	0.24	0	17,19,21	0.58	0
3	NAG	O	1	3,1	14,14,15	0.66	0	17,19,21	0.69	1 (5%)
3	NAG	O	2	3	14,14,15	0.51	0	17,19,21	0.38	0
3	BMA	O	3	3	11,11,12	0.51	0	15,15,17	0.97	1 (6%)

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	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	1/2/19/22	1/1/1/1
2	MAN	D	6	2	-	0/2/19/22	1/1/1/1
2	MAN	D	7	2	-	0/2/19/22	1/1/1/1
3	NAG	E	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
2	MAN	H	5	2	-	1/2/19/22	1/1/1/1
2	MAN	H	6	2	-	0/2/19/22	1/1/1/1
2	MAN	H	7	2	-	0/2/19/22	1/1/1/1
3	NAG	I	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	BMA	L	3	2	-	0/2/19/22	0/1/1/1
2	MAN	L	4	2	-	0/2/19/22	0/1/1/1
2	MAN	L	5	2	-	1/2/19/22	1/1/1/1
2	MAN	L	6	2	-	0/2/19/22	1/1/1/1
2	MAN	L	7	2	-	0/2/19/22	1/1/1/1
3	NAG	M	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	BMA	C3-C4-C5	3.72	116.88	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	3	BMA	C3-C4-C5	3.70	116.83	110.24
2	D	3	BMA	C3-C4-C5	3.69	116.82	110.24
2	L	1	NAG	O5-C1-C2	-3.34	106.01	111.29
2	D	1	NAG	O5-C1-C2	-3.30	106.07	111.29
2	H	1	NAG	O5-C1-C2	-3.30	106.08	111.29
2	D	6	MAN	C2-C3-C4	-2.77	106.11	110.89
2	L	6	MAN	C2-C3-C4	-2.75	106.14	110.89
2	H	6	MAN	C2-C3-C4	-2.73	106.17	110.89
2	L	3	BMA	C6-C5-C4	-2.62	106.87	113.00
2	D	3	BMA	C6-C5-C4	-2.61	106.89	113.00
2	H	3	BMA	C6-C5-C4	-2.59	106.93	113.00
2	H	7	MAN	C1-C2-C3	-2.43	106.67	109.67
2	D	7	MAN	C1-C2-C3	-2.43	106.67	109.67
2	L	7	MAN	C1-C2-C3	-2.37	106.75	109.67
2	D	3	BMA	O5-C1-C2	-2.27	107.27	110.77
2	D	4	MAN	O5-C1-C2	-2.24	107.31	110.77
2	L	3	BMA	O5-C1-C2	-2.24	107.32	110.77
3	O	3	BMA	C1-O5-C5	2.23	115.22	112.19
3	K	3	BMA	C1-O5-C5	2.23	115.21	112.19
3	G	3	BMA	C1-O5-C5	2.22	115.20	112.19
2	H	3	BMA	O5-C1-C2	-2.22	107.34	110.77
3	M	3	BMA	C1-O5-C5	2.22	115.20	112.19
2	H	4	MAN	O5-C1-C2	-2.22	107.35	110.77
3	I	3	BMA	C1-O5-C5	2.20	115.17	112.19
2	L	4	MAN	O5-C1-C2	-2.18	107.40	110.77
3	E	3	BMA	C1-O5-C5	2.17	115.14	112.19
2	H	3	BMA	O3-C3-C4	-2.13	105.44	110.35
2	D	3	BMA	O3-C3-C4	-2.12	105.45	110.35
2	L	3	BMA	O3-C3-C4	-2.11	105.48	110.35
3	K	1	NAG	C4-C3-C2	-2.06	108.00	111.02
3	G	1	NAG	C4-C3-C2	-2.04	108.03	111.02
3	O	1	NAG	C4-C3-C2	-2.04	108.03	111.02
2	D	1	NAG	C2-N2-C7	-2.01	120.04	122.90
2	L	1	NAG	C2-N2-C7	-2.01	120.05	122.90

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	H	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
4	F	1	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	D	5	MAN	O5-C5-C6-O6
2	H	5	MAN	O5-C5-C6-O6
2	L	5	MAN	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	L	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
3	G	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6

All (9) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	7	MAN	C1-C2-C3-C4-C5-O5
2	H	7	MAN	C1-C2-C3-C4-C5-O5

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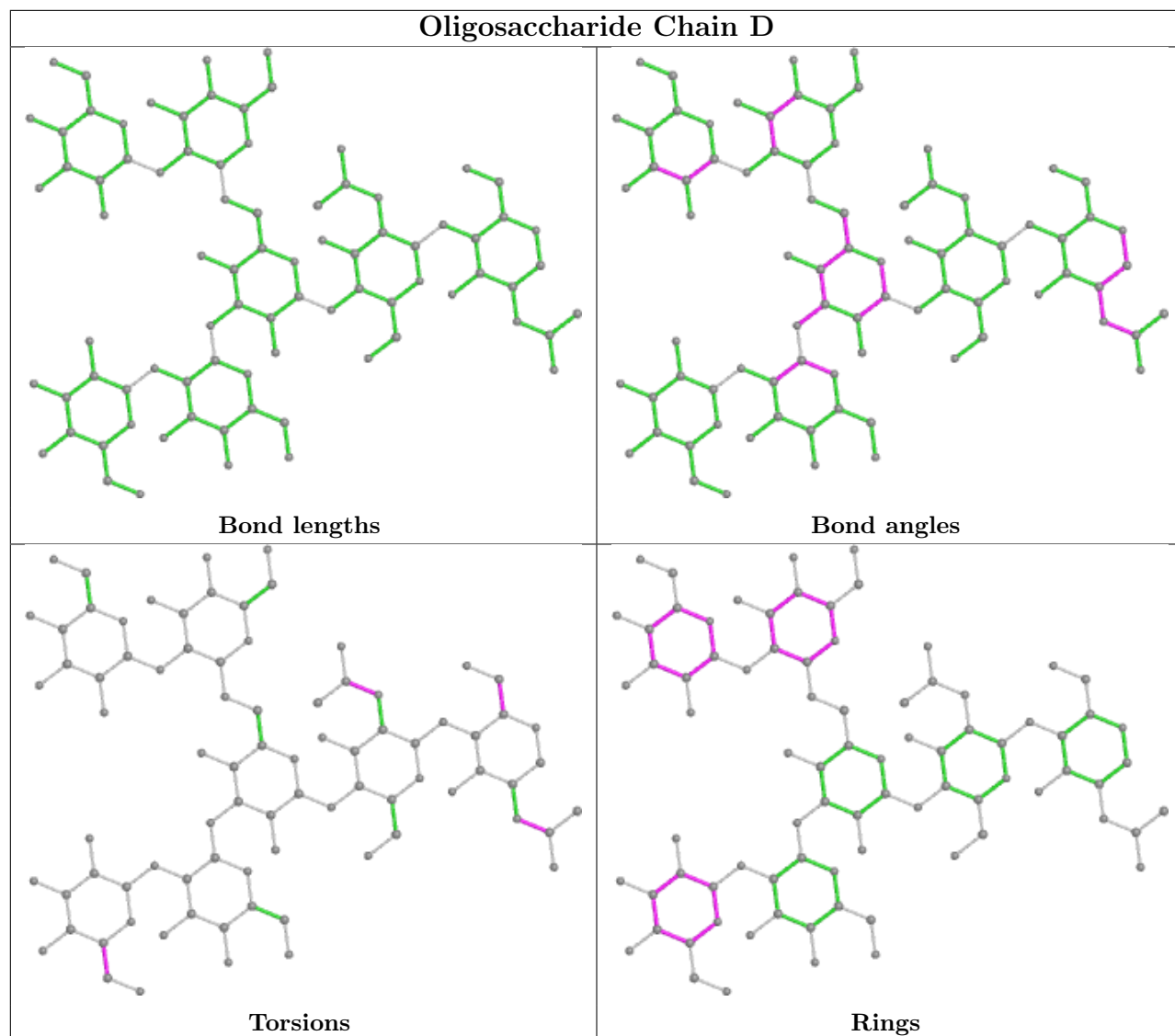
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Mol	Chain	Res	Type	Atoms
2	L	7	MAN	C1-C2-C3-C4-C5-O5
2	H	5	MAN	C1-C2-C3-C4-C5-O5
2	L	5	MAN	C1-C2-C3-C4-C5-O5
2	D	5	MAN	C1-C2-C3-C4-C5-O5
2	H	6	MAN	C1-C2-C3-C4-C5-O5
2	D	6	MAN	C1-C2-C3-C4-C5-O5
2	L	6	MAN	C1-C2-C3-C4-C5-O5

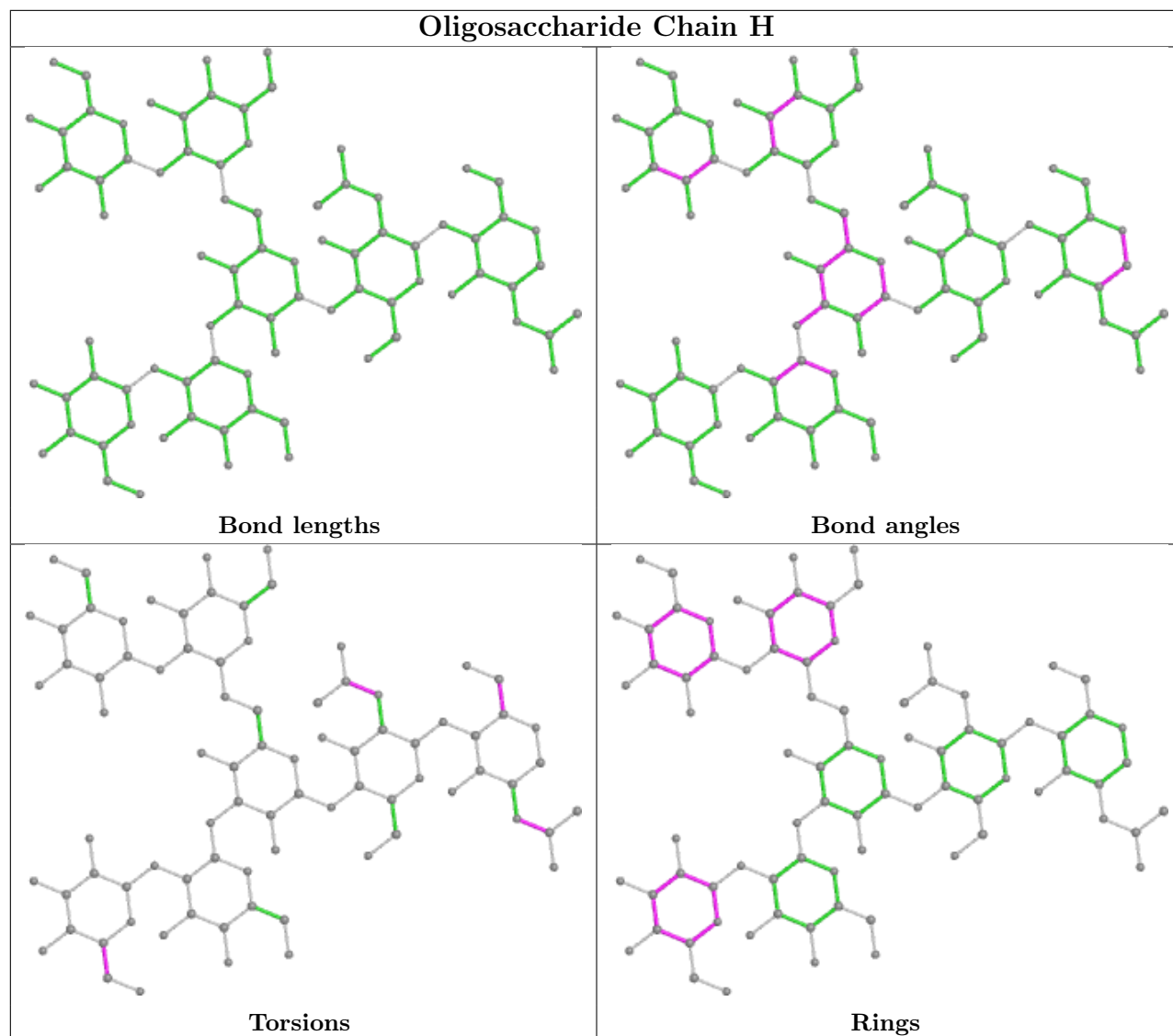
3 monomers are involved in 6 short contacts:

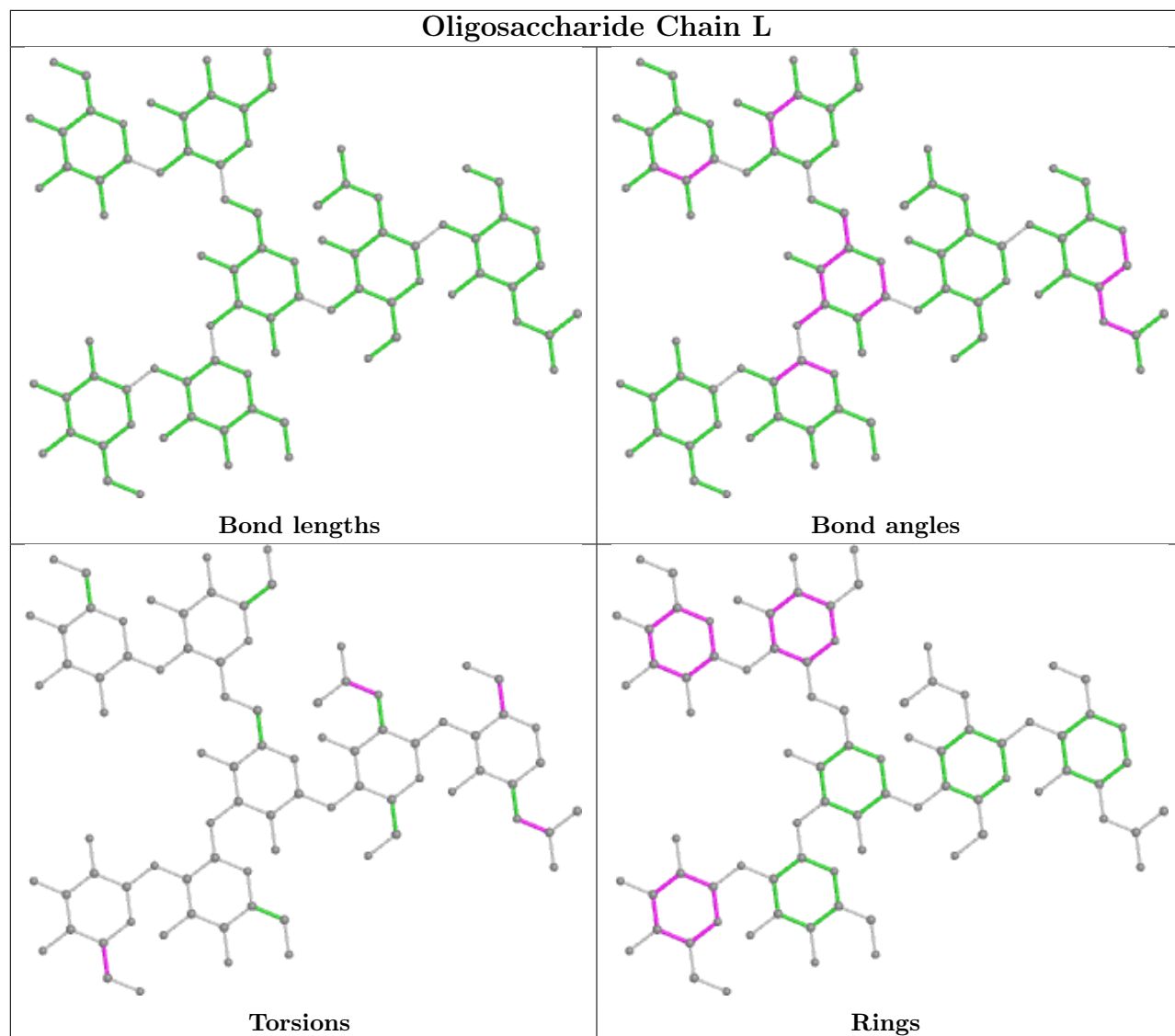
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1	NAG	2	0
3	K	1	NAG	2	0
3	G	1	NAG	2	0

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

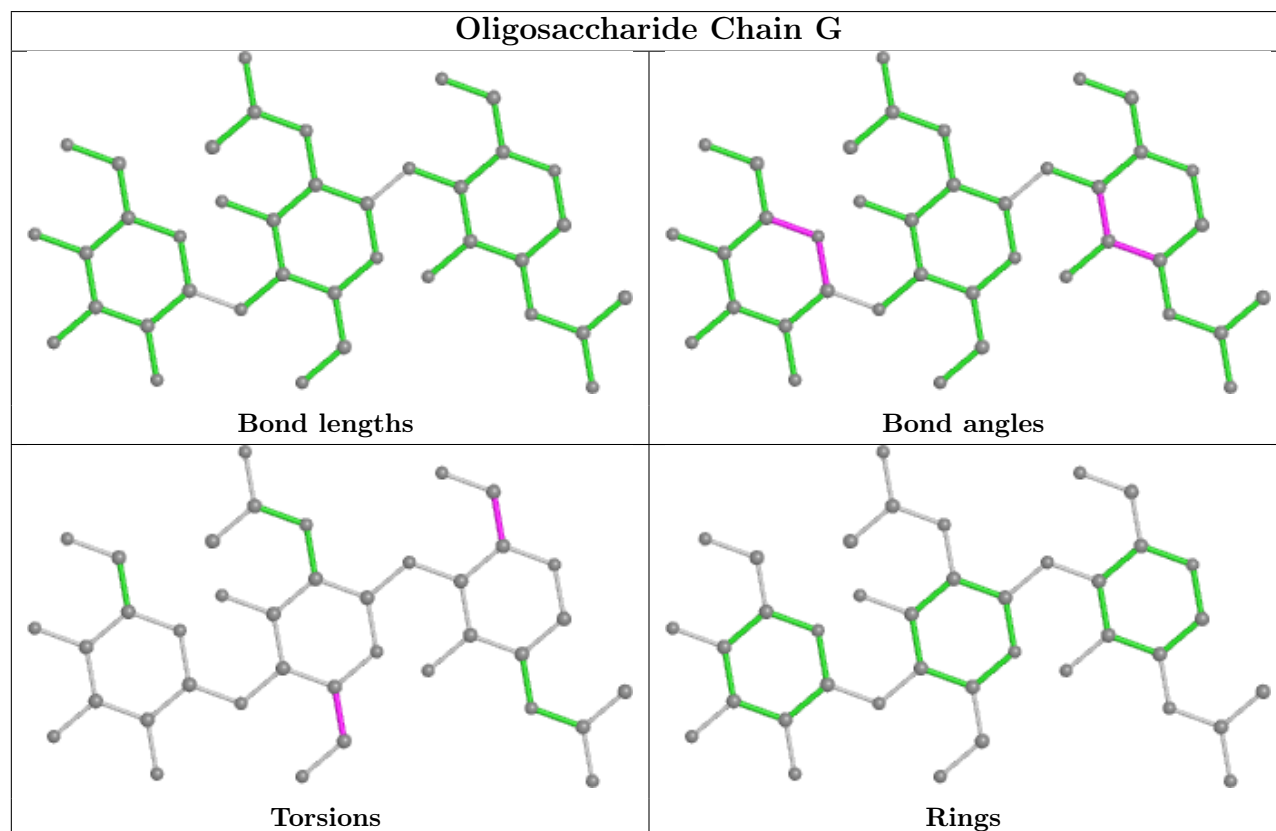
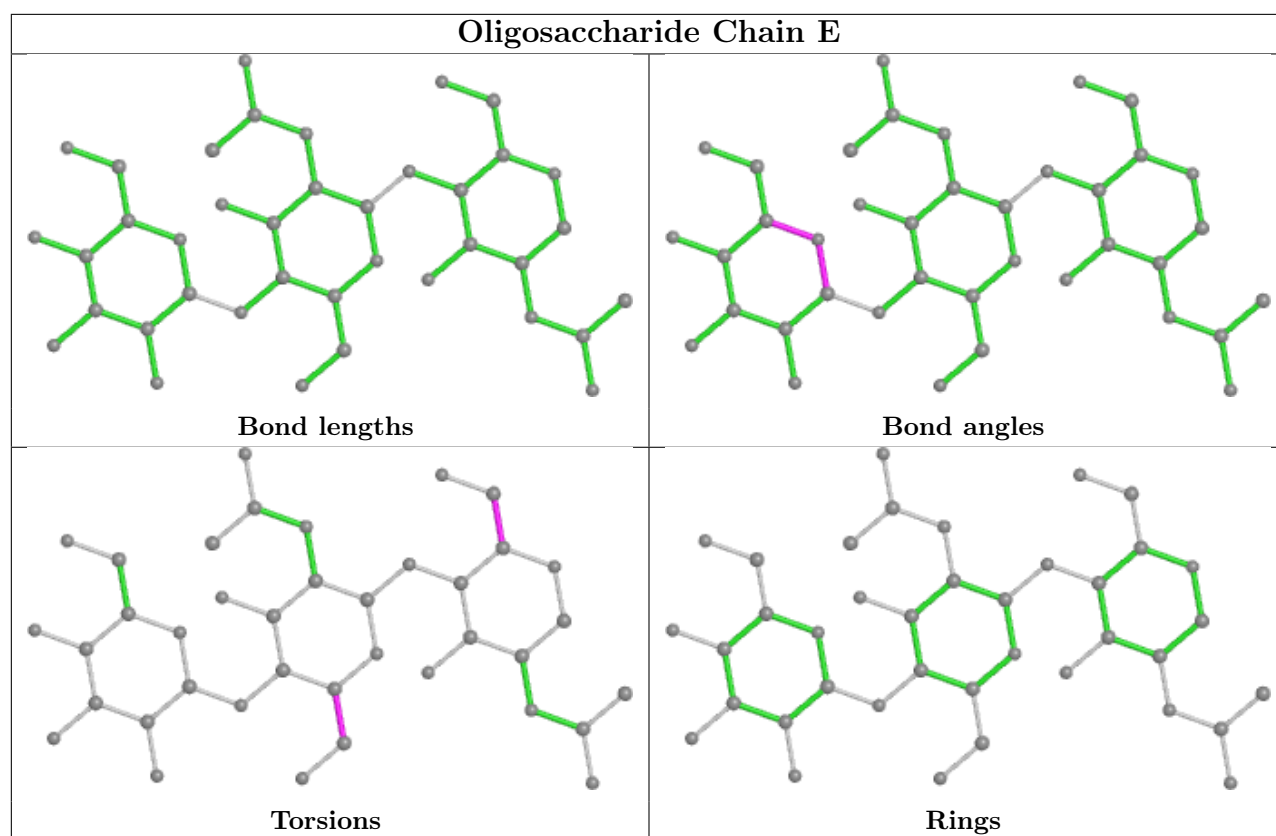


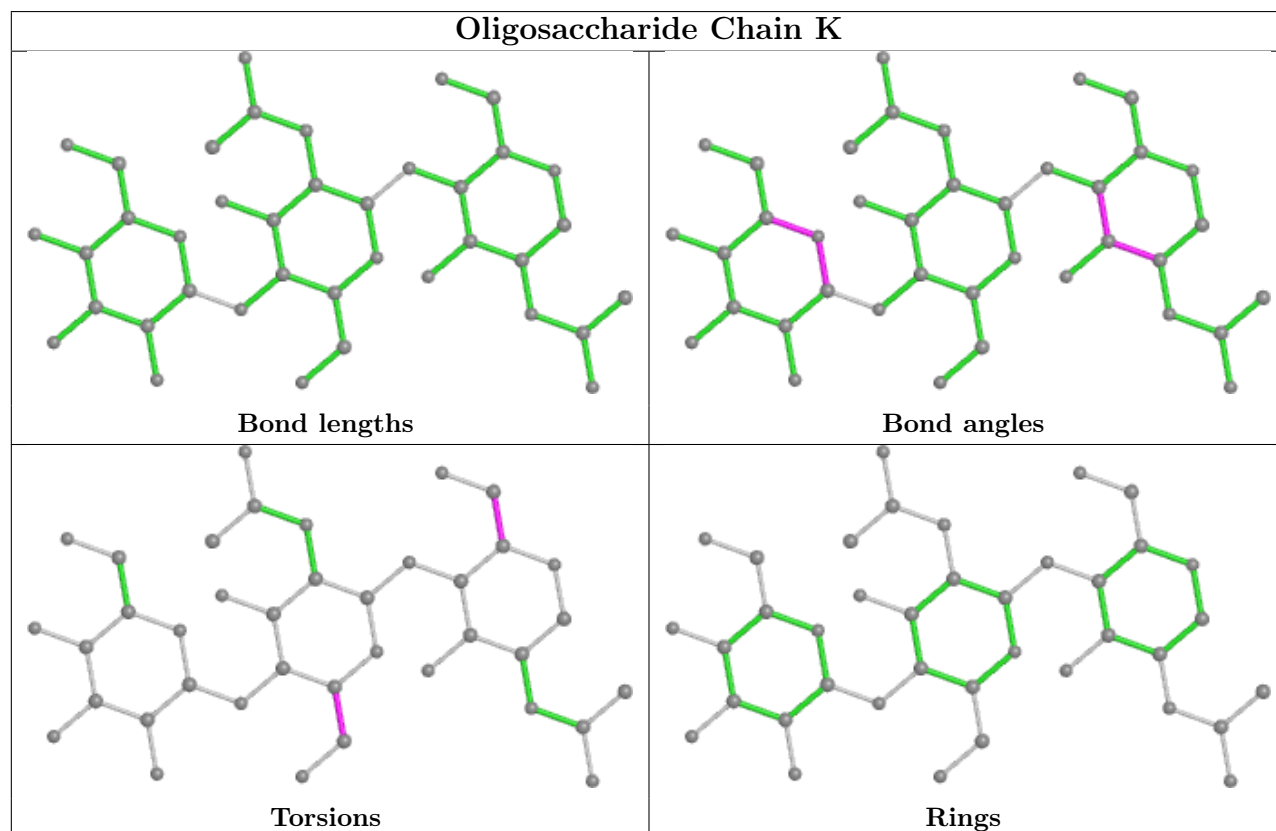
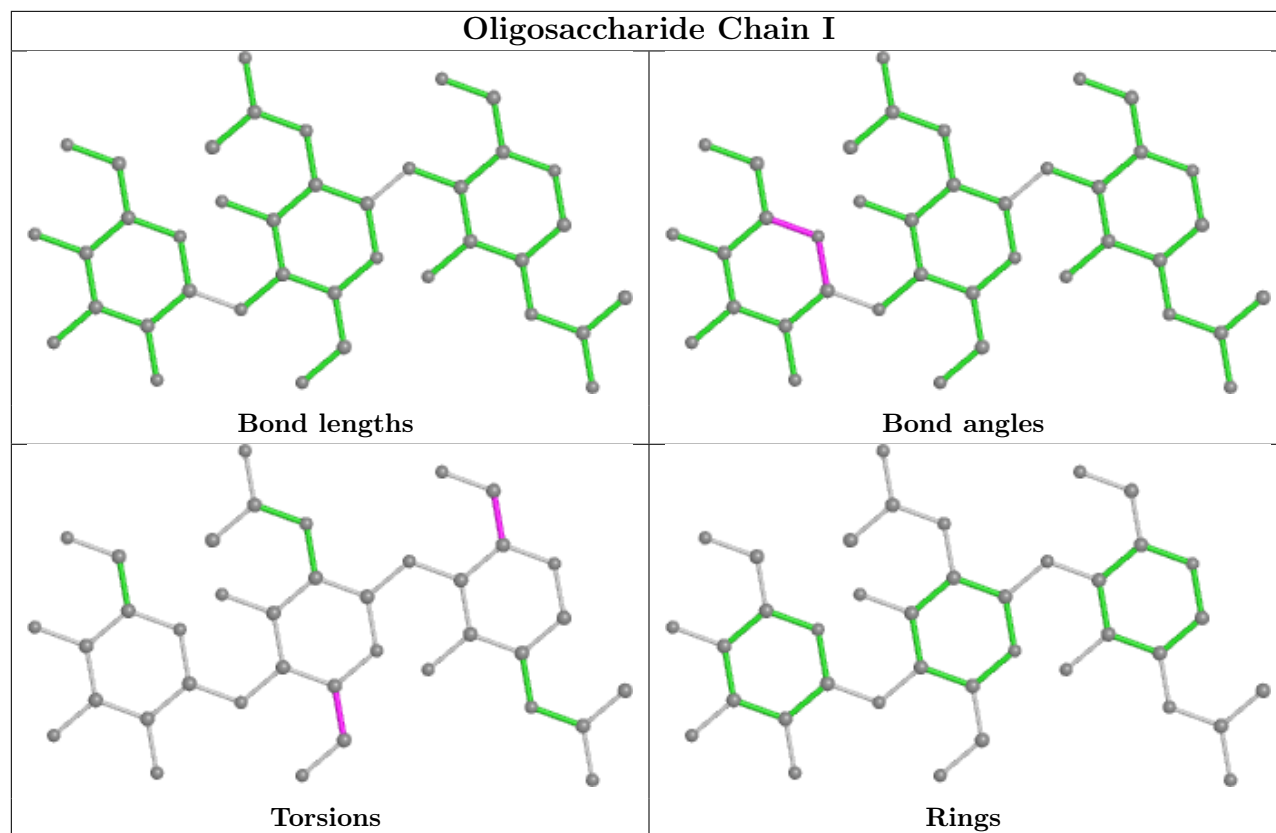
## Oligosaccharide Chain H

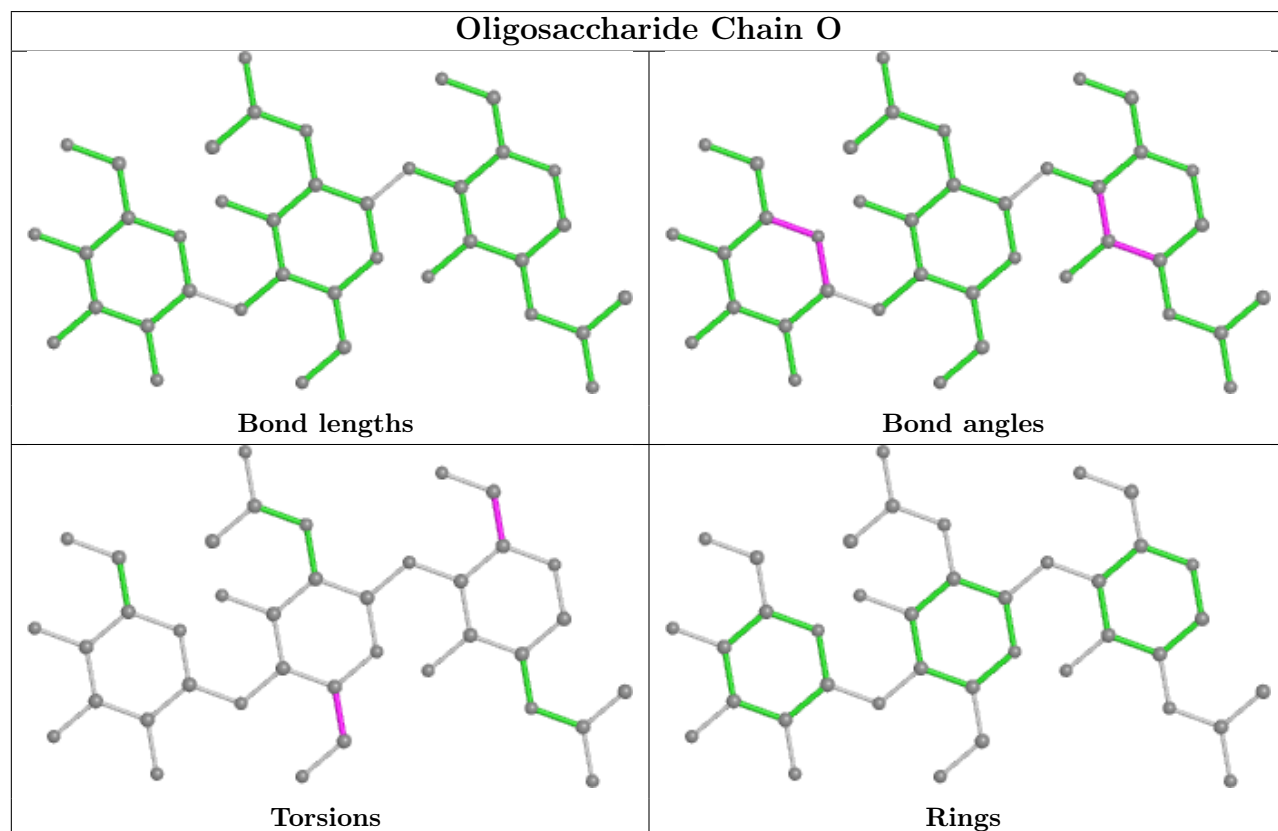
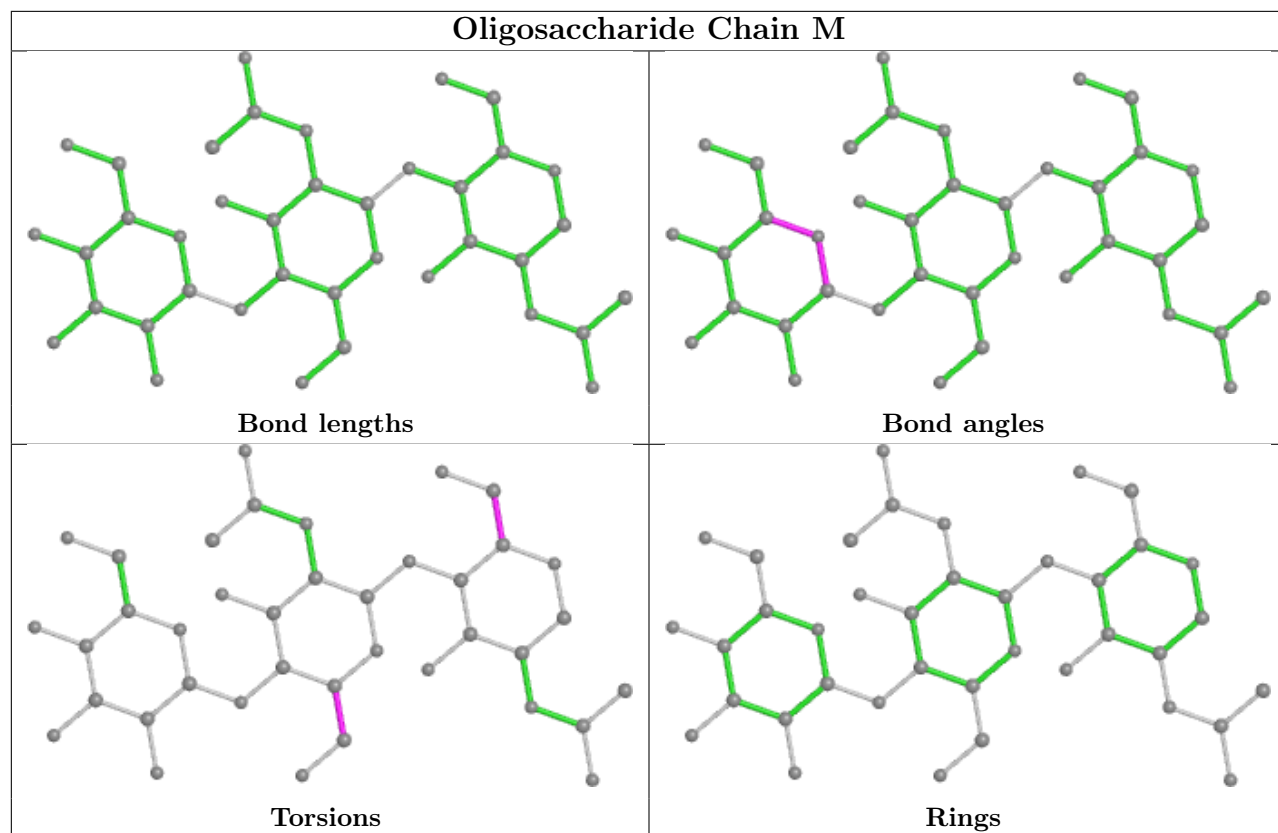


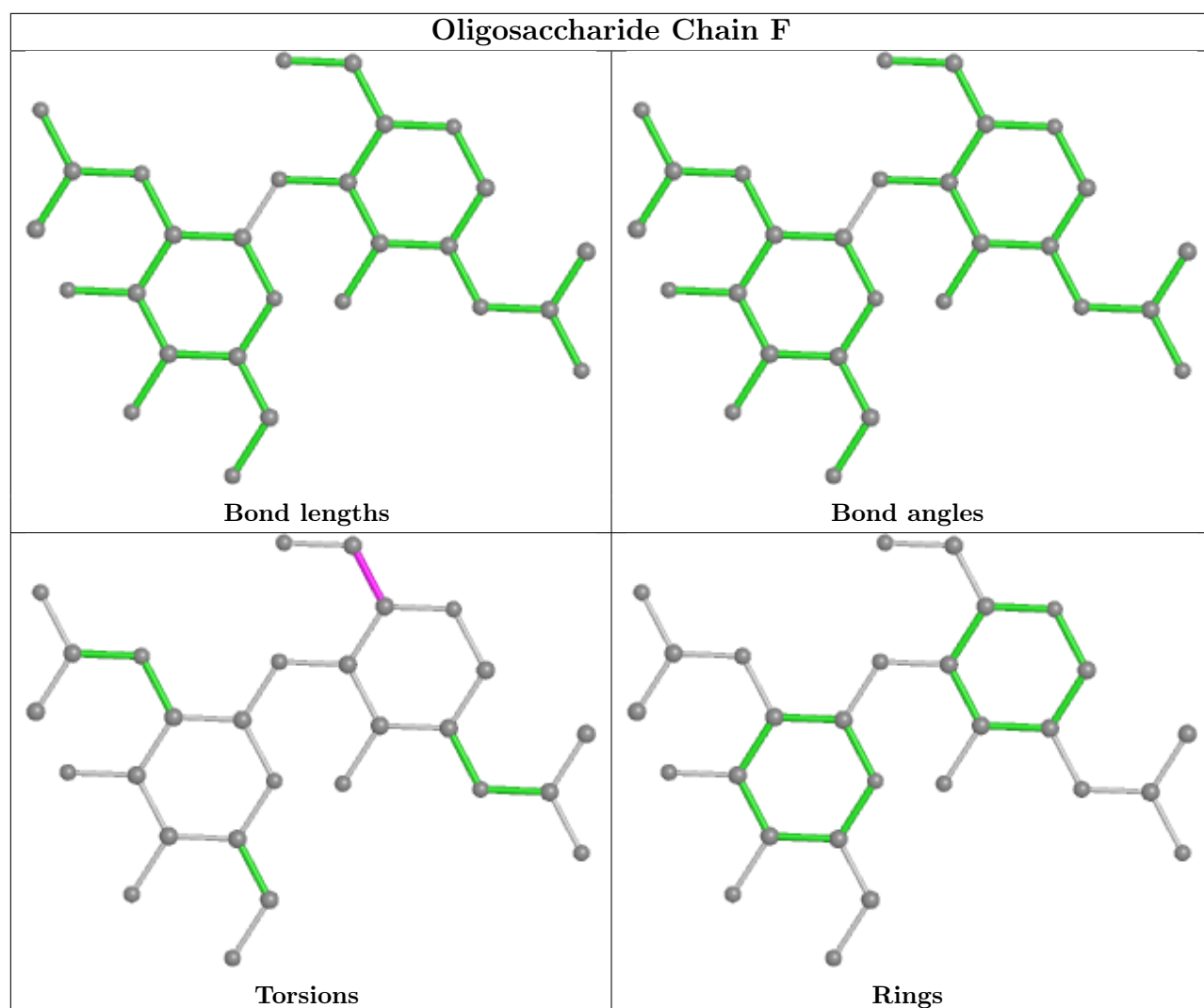


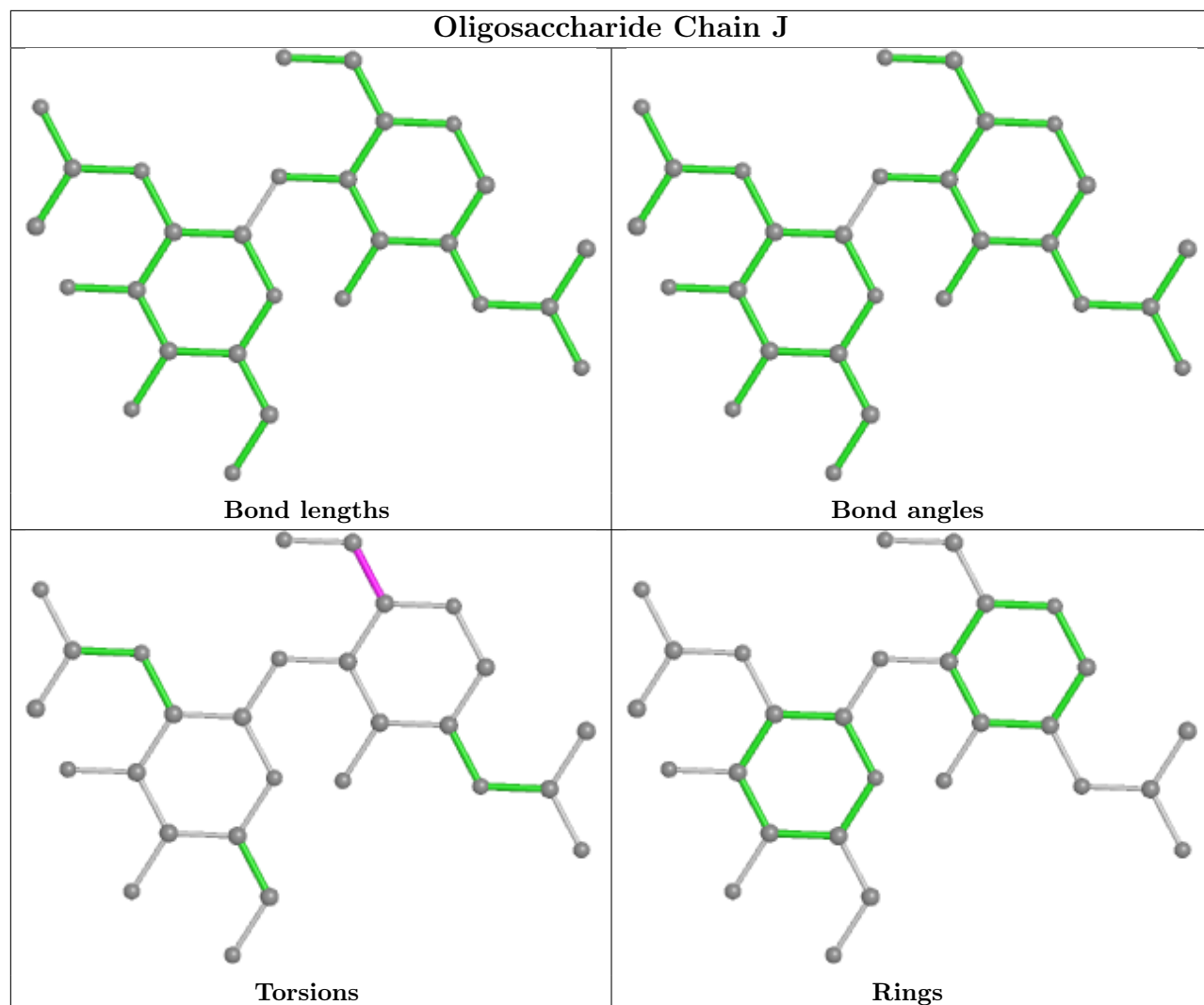


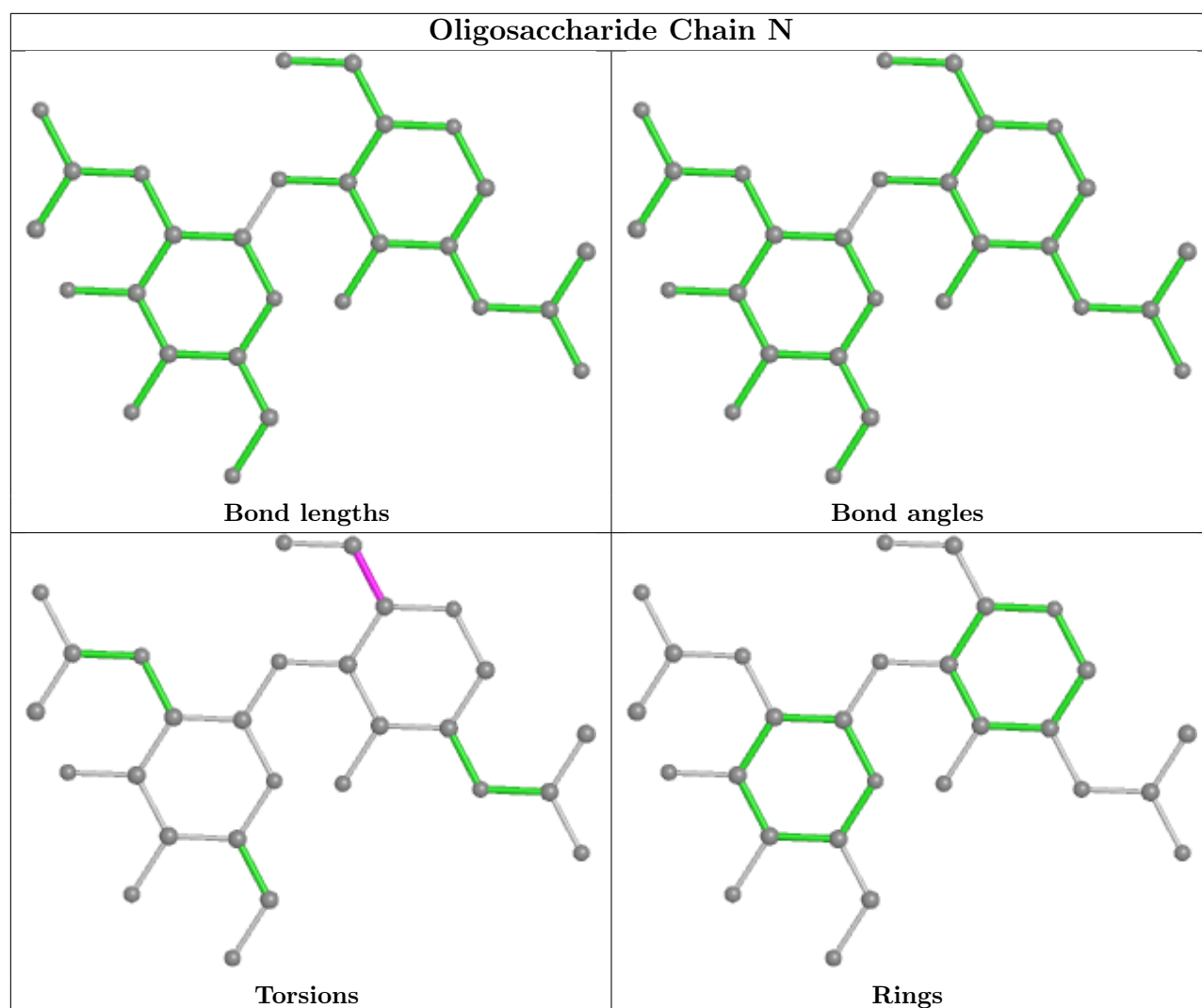












## 5.6 Ligand geometry [i](#)

48 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	B	1208	1	14,14,15	0.13	0	17,19,21	0.60	0
5	NAG	C	1216	1	14,14,15	0.52	0	17,19,21	0.39	0
5	NAG	A	1204	1	14,14,15	0.22	0	17,19,21	0.35	0
5	NAG	C	1206	1	14,14,15	0.19	0	17,19,21	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1216	1	14,14,15	0.50	0	17,19,21	0.39	0
5	NAG	B	1213	1	14,14,15	0.22	0	17,19,21	0.73	1 (5%)
5	NAG	C	1202	1	14,14,15	0.59	0	17,19,21	0.45	0
5	NAG	B	1202	1	14,14,15	0.61	0	17,19,21	0.46	0
5	NAG	C	1208	1	14,14,15	0.13	0	17,19,21	0.60	0
5	NAG	A	1210	1	14,14,15	0.31	0	17,19,21	0.47	0
5	NAG	B	1209	1	14,14,15	0.78	1 (7%)	17,19,21	0.43	0
5	NAG	A	1202	1	14,14,15	0.60	0	17,19,21	0.46	0
5	NAG	A	1203	1	14,14,15	0.27	0	17,19,21	0.40	0
5	NAG	A	1207	1	14,14,15	0.28	0	17,19,21	0.83	1 (5%)
5	NAG	B	1201	1	14,14,15	0.55	0	17,19,21	0.46	0
5	NAG	A	1208	1	14,14,15	0.13	0	17,19,21	0.59	0
5	NAG	A	1201	1	14,14,15	0.55	0	17,19,21	0.47	0
5	NAG	B	1215	1	14,14,15	0.37	0	17,19,21	0.32	0
5	NAG	C	1211	1	14,14,15	1.22	1 (7%)	17,19,21	1.69	2 (11%)
5	NAG	B	1210	1	14,14,15	0.31	0	17,19,21	0.45	0
5	NAG	C	1214	1	14,14,15	0.33	0	17,19,21	0.63	1 (5%)
5	NAG	A	1212	1	14,14,15	0.27	0	17,19,21	0.36	0
5	NAG	A	1211	1	14,14,15	1.22	1 (7%)	17,19,21	1.68	2 (11%)
5	NAG	C	1203	1	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	A	1214	1	14,14,15	0.32	0	17,19,21	0.65	1 (5%)
5	NAG	A	1205	1	14,14,15	0.37	0	17,19,21	0.78	1 (5%)
5	NAG	A	1213	1	14,14,15	0.21	0	17,19,21	0.73	1 (5%)
5	NAG	C	1205	1	14,14,15	0.38	0	17,19,21	0.77	1 (5%)
5	NAG	B	1211	1	14,14,15	1.19	1 (7%)	17,19,21	1.68	2 (11%)
5	NAG	B	1214	1	14,14,15	0.31	0	17,19,21	0.63	1 (5%)
5	NAG	A	1206	1	14,14,15	0.21	0	17,19,21	0.36	0
5	NAG	B	1204	1	14,14,15	0.23	0	17,19,21	0.36	0
5	NAG	C	1210	1	14,14,15	0.31	0	17,19,21	0.46	0
5	NAG	C	1201	1	14,14,15	0.56	0	17,19,21	0.46	0
5	NAG	B	1216	1	14,14,15	0.51	0	17,19,21	0.39	0
5	NAG	B	1203	1	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	C	1209	1	14,14,15	0.80	1 (7%)	17,19,21	0.43	0
5	NAG	C	1212	1	14,14,15	0.28	0	17,19,21	0.35	0
5	NAG	B	1207	1	14,14,15	0.29	0	17,19,21	0.82	1 (5%)
5	NAG	B	1205	1	14,14,15	0.38	0	17,19,21	0.78	1 (5%)
5	NAG	B	1212	1	14,14,15	0.26	0	17,19,21	0.37	0
5	NAG	C	1215	1	14,14,15	0.36	0	17,19,21	0.32	0
5	NAG	C	1207	1	14,14,15	0.29	0	17,19,21	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1209	1	14,14,15	0.79	1 (7%)	17,19,21	0.42	0
5	NAG	B	1206	1	14,14,15	0.21	0	17,19,21	0.35	0
5	NAG	C	1204	1	14,14,15	0.23	0	17,19,21	0.37	0
5	NAG	A	1215	1	14,14,15	0.37	0	17,19,21	0.32	0
5	NAG	C	1213	1	14,14,15	0.20	0	17,19,21	0.73	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
5	NAG	B	1208	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1216	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1204	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1206	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1216	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1213	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1202	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1202	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1208	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1210	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1209	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1202	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1203	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1207	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1201	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1208	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1201	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1215	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1211	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1210	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1214	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1212	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1211	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1203	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1214	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1205	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1213	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1205	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1211	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1214	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1206	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1204	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1210	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1201	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1216	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1203	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1209	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1212	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1207	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1205	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1212	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1215	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1207	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1209	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1206	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1204	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1215	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1213	1	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1211	NAG	C1-C2	4.11	1.58	1.52
5	A	1211	NAG	C1-C2	4.11	1.58	1.52
5	B	1211	NAG	C1-C2	3.99	1.58	1.52
5	C	1209	NAG	O5-C1	-2.67	1.39	1.43
5	A	1209	NAG	O5-C1	-2.64	1.39	1.43
5	B	1209	NAG	O5-C1	-2.58	1.39	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1211	NAG	C1-O5-C5	5.64	119.84	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1211	NAG	C1-O5-C5	5.60	119.78	112.19
5	B	1211	NAG	C1-O5-C5	5.60	119.78	112.19
5	C	1211	NAG	C4-C3-C2	3.59	116.28	111.02
5	A	1211	NAG	C4-C3-C2	3.56	116.24	111.02
5	B	1211	NAG	C4-C3-C2	3.55	116.23	111.02
5	A	1207	NAG	C1-O5-C5	3.05	116.32	112.19
5	B	1207	NAG	C1-O5-C5	3.04	116.31	112.19
5	C	1207	NAG	C1-O5-C5	3.01	116.27	112.19
5	C	1213	NAG	C1-O5-C5	2.56	115.66	112.19
5	B	1213	NAG	C1-O5-C5	2.54	115.64	112.19
5	A	1213	NAG	C1-O5-C5	2.53	115.62	112.19
5	B	1205	NAG	C1-O5-C5	2.16	115.12	112.19
5	A	1205	NAG	C1-O5-C5	2.13	115.08	112.19
5	C	1205	NAG	C1-O5-C5	2.11	115.05	112.19
5	A	1214	NAG	C1-O5-C5	2.06	114.98	112.19
5	C	1214	NAG	C1-O5-C5	2.02	114.94	112.19
5	B	1214	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1214	NAG	C4-C5-C6-O6
5	A	1214	NAG	C4-C5-C6-O6
5	B	1214	NAG	C4-C5-C6-O6
5	A	1208	NAG	O5-C5-C6-O6
5	B	1208	NAG	O5-C5-C6-O6
5	C	1208	NAG	O5-C5-C6-O6
5	A	1209	NAG	O5-C5-C6-O6
5	A	1211	NAG	O5-C5-C6-O6
5	B	1209	NAG	O5-C5-C6-O6
5	B	1211	NAG	O5-C5-C6-O6
5	C	1209	NAG	O5-C5-C6-O6
5	C	1211	NAG	O5-C5-C6-O6
5	A	1212	NAG	C4-C5-C6-O6
5	B	1212	NAG	C4-C5-C6-O6
5	C	1212	NAG	C4-C5-C6-O6
5	A	1205	NAG	O5-C5-C6-O6
5	A	1206	NAG	O5-C5-C6-O6
5	A	1212	NAG	O5-C5-C6-O6
5	B	1205	NAG	O5-C5-C6-O6
5	B	1206	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1212	NAG	O5-C5-C6-O6
5	C	1206	NAG	O5-C5-C6-O6
5	C	1212	NAG	O5-C5-C6-O6
5	C	1205	NAG	O5-C5-C6-O6
5	A	1214	NAG	O5-C5-C6-O6
5	B	1214	NAG	O5-C5-C6-O6
5	C	1214	NAG	O5-C5-C6-O6
5	A	1201	NAG	C1-C2-N2-C7
5	B	1201	NAG	C1-C2-N2-C7
5	C	1201	NAG	C1-C2-N2-C7
5	A	1209	NAG	C4-C5-C6-O6
5	B	1209	NAG	C4-C5-C6-O6
5	C	1209	NAG	C4-C5-C6-O6
5	A	1205	NAG	C4-C5-C6-O6
5	A	1211	NAG	C4-C5-C6-O6
5	B	1205	NAG	C4-C5-C6-O6
5	B	1211	NAG	C4-C5-C6-O6
5	C	1205	NAG	C4-C5-C6-O6
5	C	1211	NAG	C4-C5-C6-O6
5	A	1208	NAG	C4-C5-C6-O6
5	B	1208	NAG	C4-C5-C6-O6
5	C	1208	NAG	C4-C5-C6-O6
5	A	1202	NAG	C8-C7-N2-C2
5	A	1202	NAG	O7-C7-N2-C2
5	A	1203	NAG	C8-C7-N2-C2
5	A	1203	NAG	O7-C7-N2-C2
5	A	1215	NAG	C8-C7-N2-C2
5	A	1215	NAG	O7-C7-N2-C2
5	A	1216	NAG	C8-C7-N2-C2
5	A	1216	NAG	O7-C7-N2-C2
5	B	1202	NAG	C8-C7-N2-C2
5	B	1202	NAG	O7-C7-N2-C2
5	B	1203	NAG	C8-C7-N2-C2
5	B	1203	NAG	O7-C7-N2-C2
5	B	1215	NAG	C8-C7-N2-C2
5	B	1215	NAG	O7-C7-N2-C2
5	B	1216	NAG	C8-C7-N2-C2
5	B	1216	NAG	O7-C7-N2-C2
5	C	1202	NAG	C8-C7-N2-C2
5	C	1202	NAG	O7-C7-N2-C2
5	C	1203	NAG	C8-C7-N2-C2
5	C	1203	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	C	1215	NAG	C8-C7-N2-C2
5	C	1215	NAG	O7-C7-N2-C2
5	C	1216	NAG	C8-C7-N2-C2
5	C	1216	NAG	O7-C7-N2-C2
5	A	1202	NAG	O5-C5-C6-O6
5	B	1202	NAG	O5-C5-C6-O6
5	C	1202	NAG	O5-C5-C6-O6
5	B	1206	NAG	C4-C5-C6-O6
5	C	1206	NAG	C4-C5-C6-O6
5	A	1206	NAG	C4-C5-C6-O6
5	A	1215	NAG	O5-C5-C6-O6
5	B	1215	NAG	O5-C5-C6-O6
5	C	1215	NAG	O5-C5-C6-O6
5	A	1213	NAG	C4-C5-C6-O6
5	B	1213	NAG	C4-C5-C6-O6
5	A	1216	NAG	C4-C5-C6-O6
5	C	1213	NAG	C4-C5-C6-O6
5	C	1216	NAG	C4-C5-C6-O6
5	B	1216	NAG	C4-C5-C6-O6
5	B	1213	NAG	O5-C5-C6-O6
5	A	1210	NAG	O5-C5-C6-O6
5	A	1213	NAG	O5-C5-C6-O6
5	B	1210	NAG	O5-C5-C6-O6
5	C	1210	NAG	O5-C5-C6-O6
5	C	1213	NAG	O5-C5-C6-O6
5	B	1210	NAG	C4-C5-C6-O6
5	A	1210	NAG	C4-C5-C6-O6
5	C	1210	NAG	C4-C5-C6-O6
5	A	1201	NAG	C3-C2-N2-C7
5	A	1205	NAG	C3-C2-N2-C7
5	A	1208	NAG	C3-C2-N2-C7
5	B	1201	NAG	C3-C2-N2-C7
5	B	1205	NAG	C3-C2-N2-C7
5	B	1208	NAG	C3-C2-N2-C7
5	C	1201	NAG	C3-C2-N2-C7
5	C	1205	NAG	C3-C2-N2-C7
5	C	1208	NAG	C3-C2-N2-C7

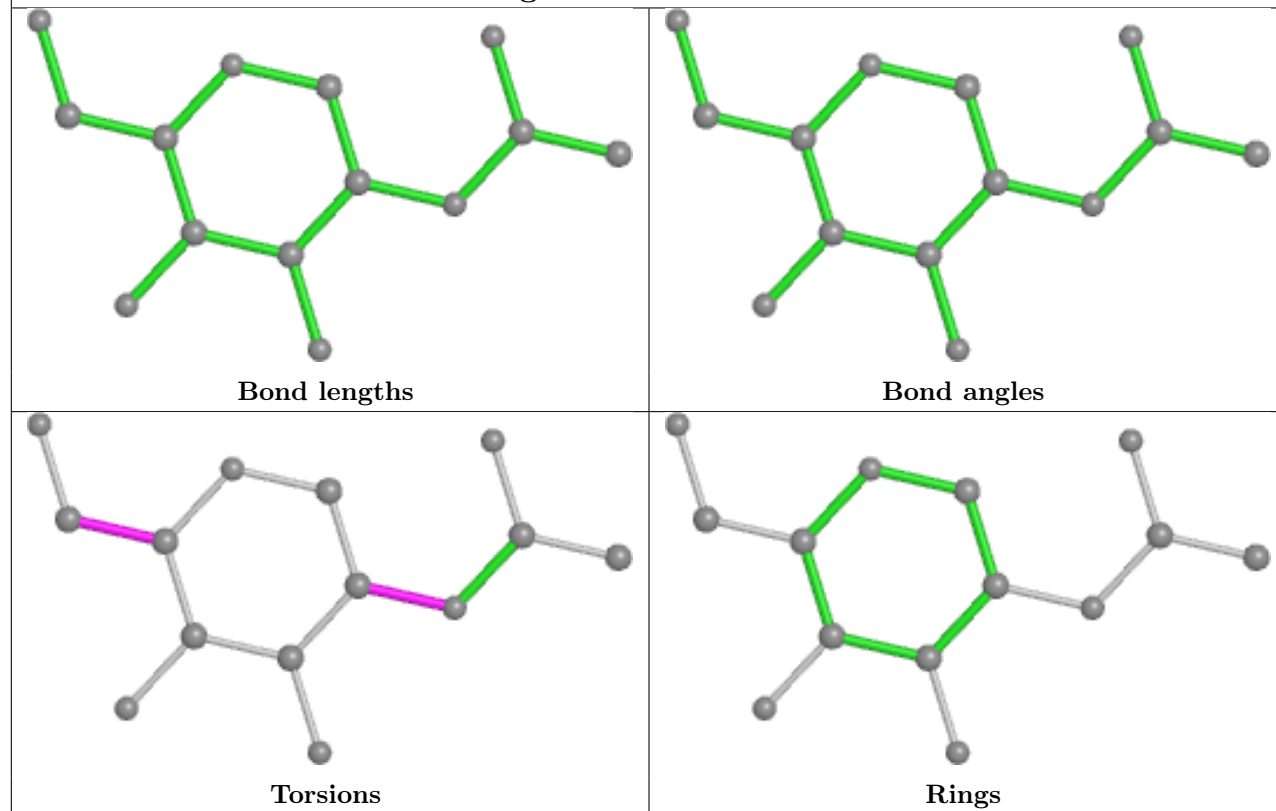
There are no ring outliers.

11 monomers are involved in 44 short contacts:

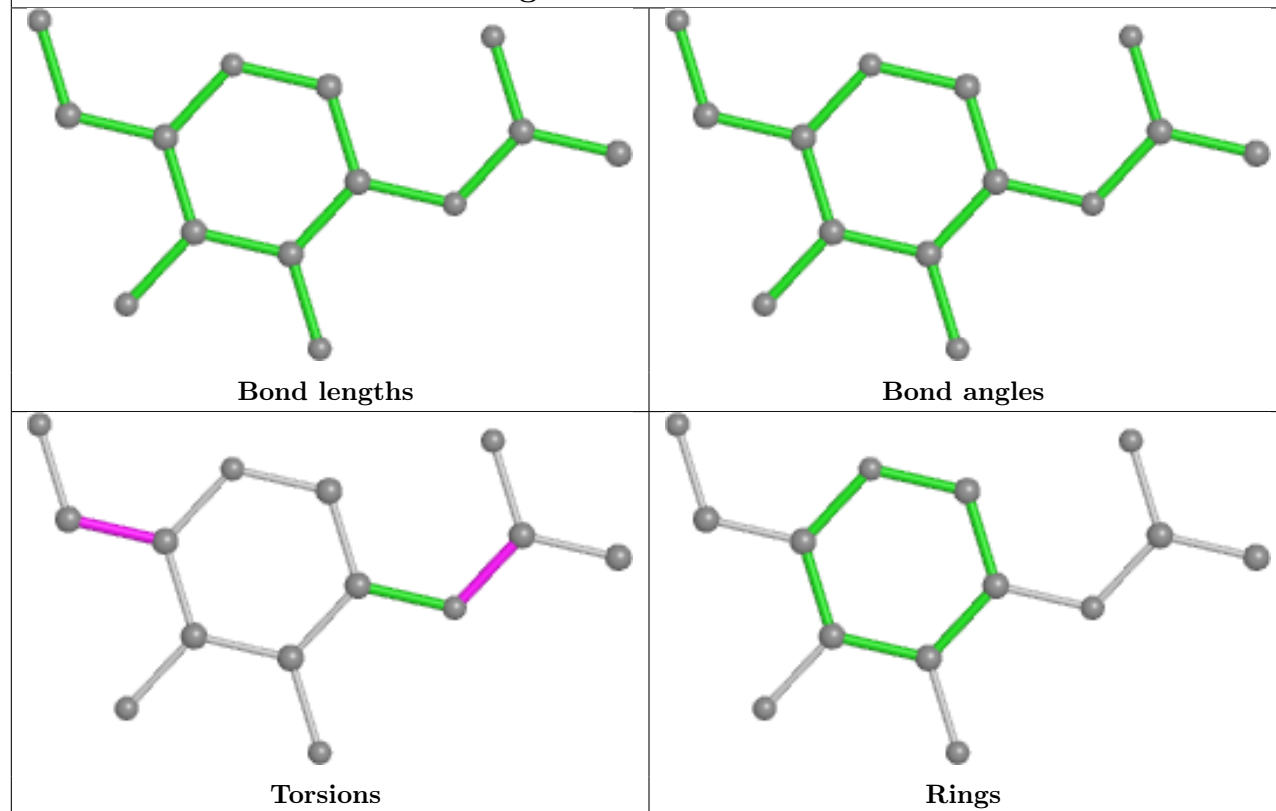
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1216	NAG	1	0
5	C	1202	NAG	6	0
5	B	1202	NAG	6	0
5	A	1202	NAG	4	0
5	B	1201	NAG	7	0
5	A	1201	NAG	8	0
5	A	1205	NAG	1	0
5	C	1205	NAG	1	0
5	A	1206	NAG	1	0
5	C	1201	NAG	8	0
5	B	1205	NAG	1	0

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

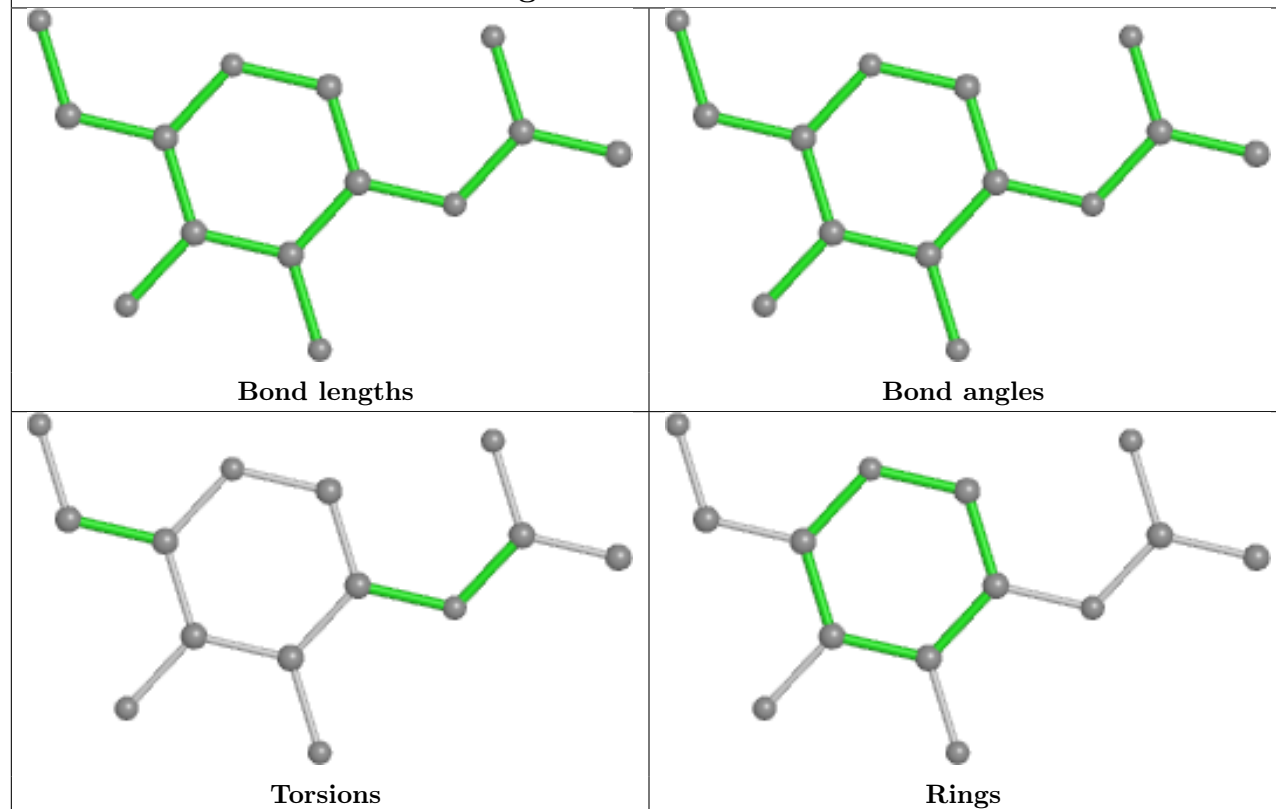
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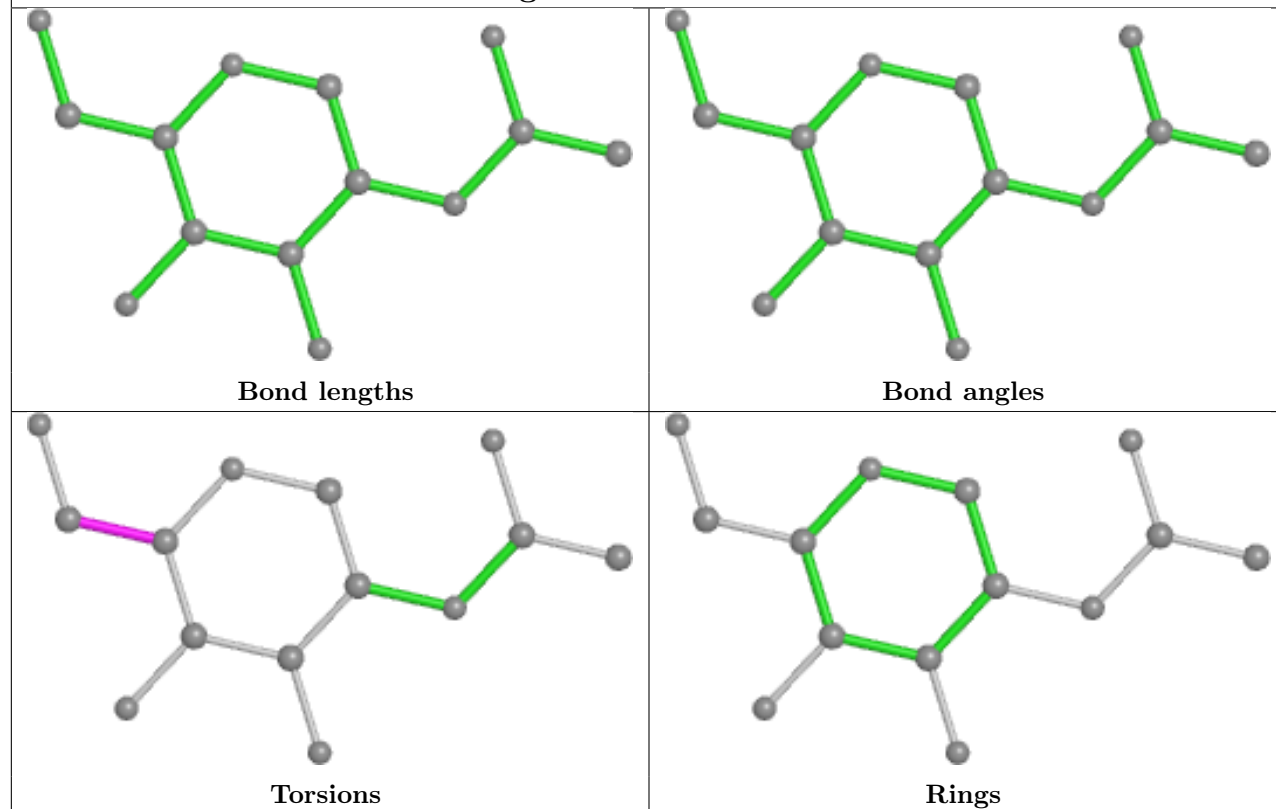
## Ligand NAG C 1216



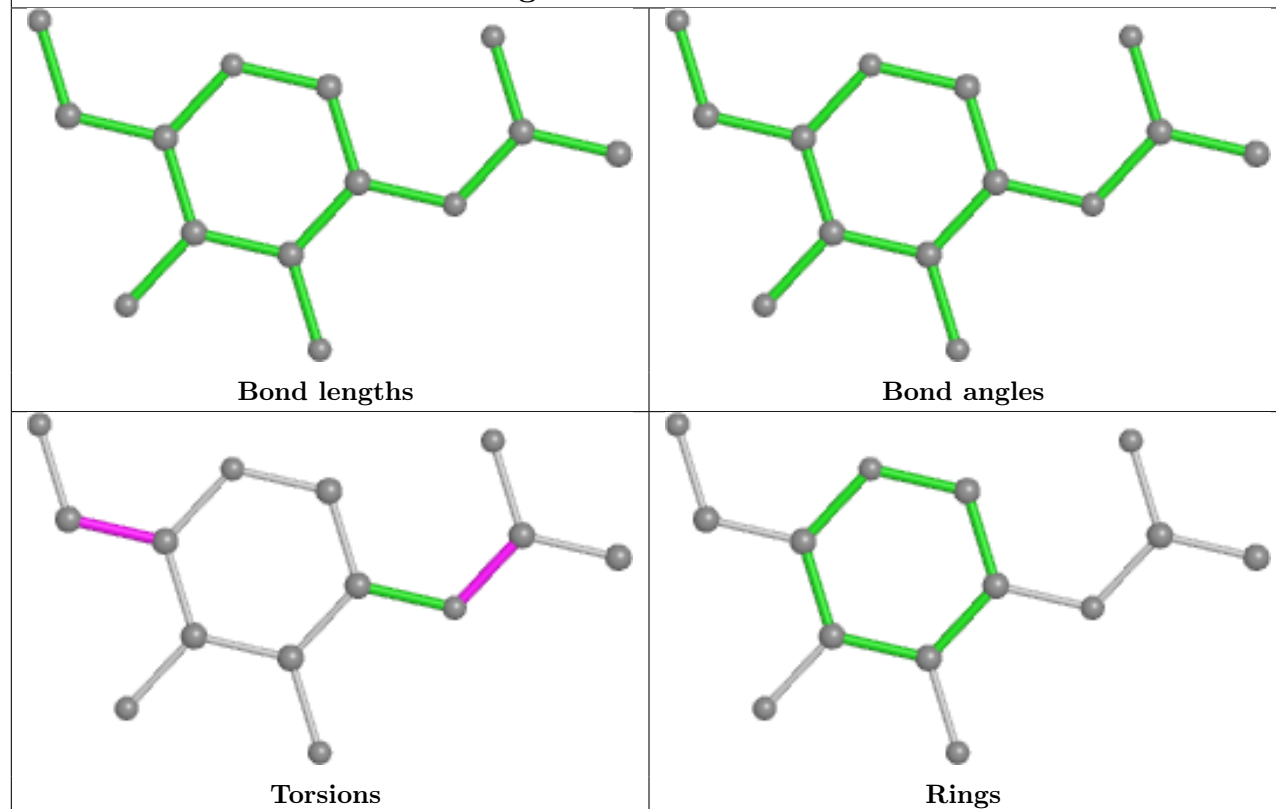
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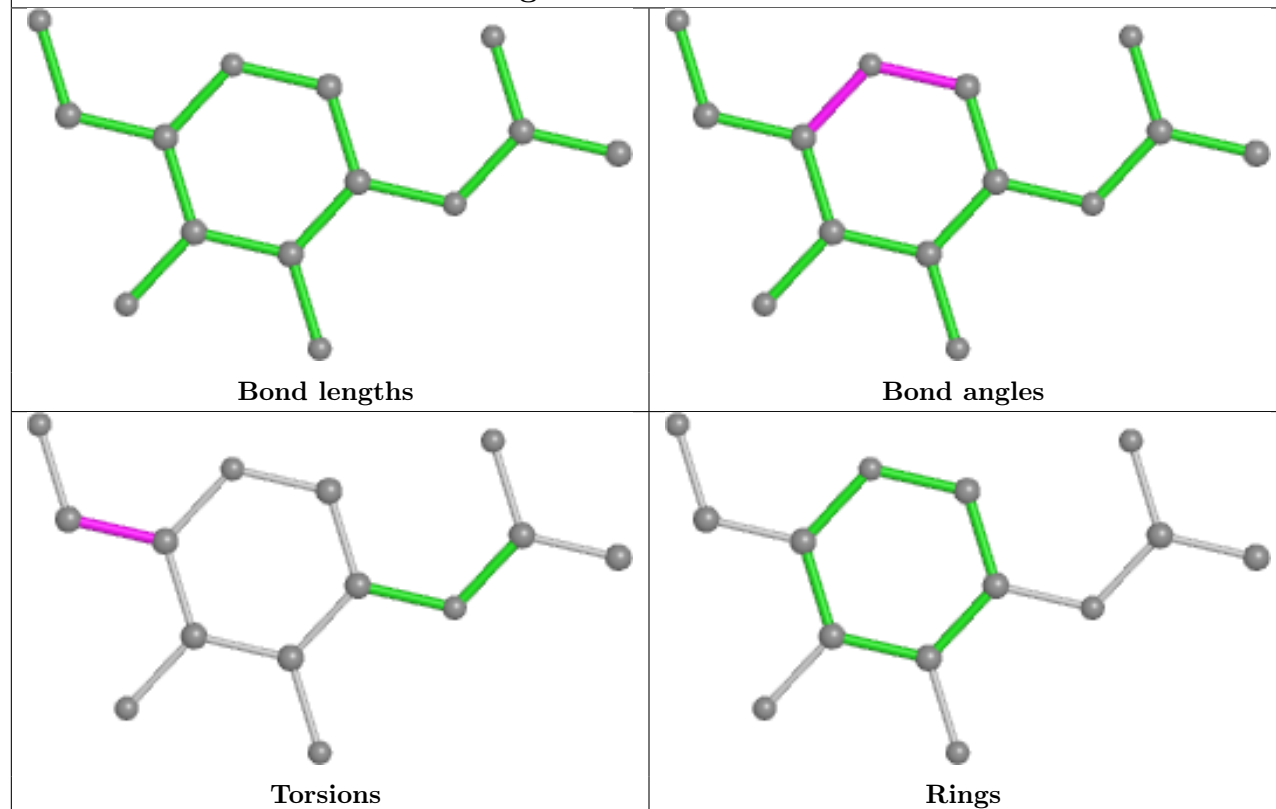
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## Ligand NAG A 1216

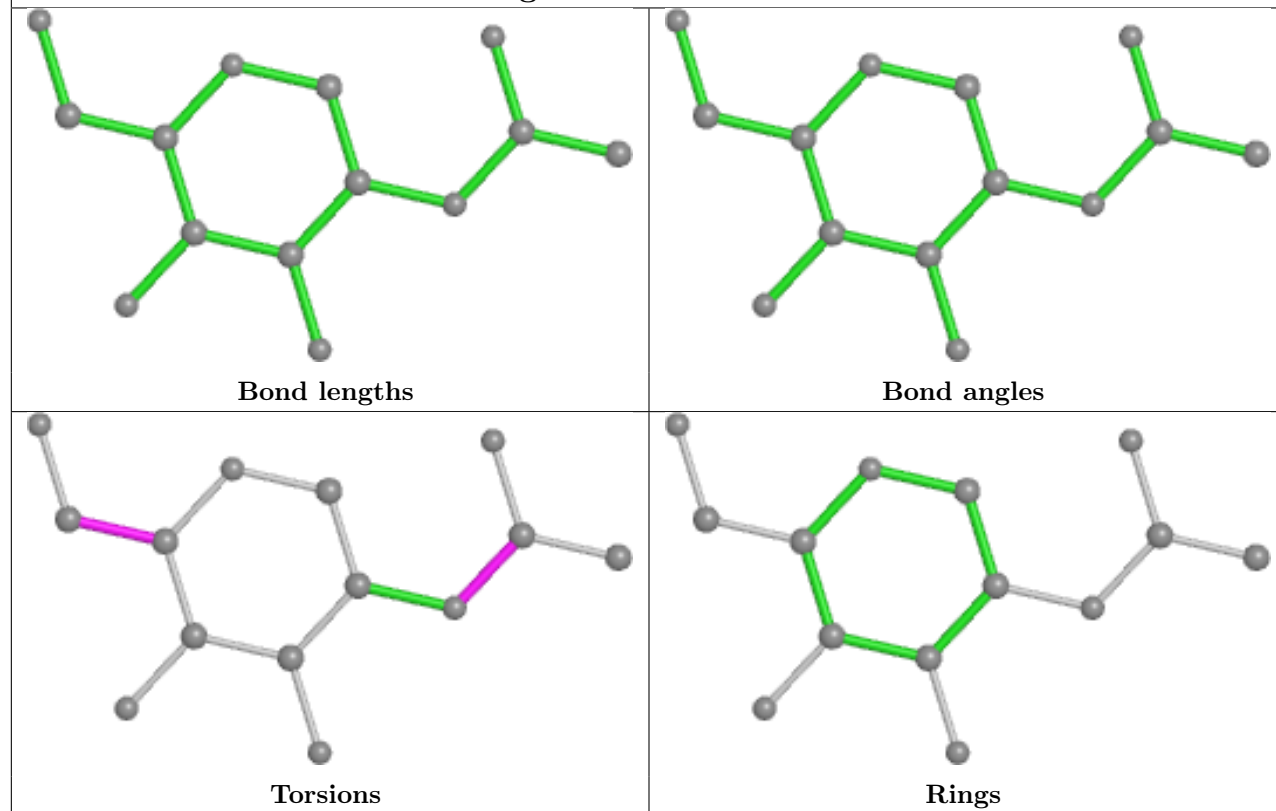


## Ligand NAG B 1213

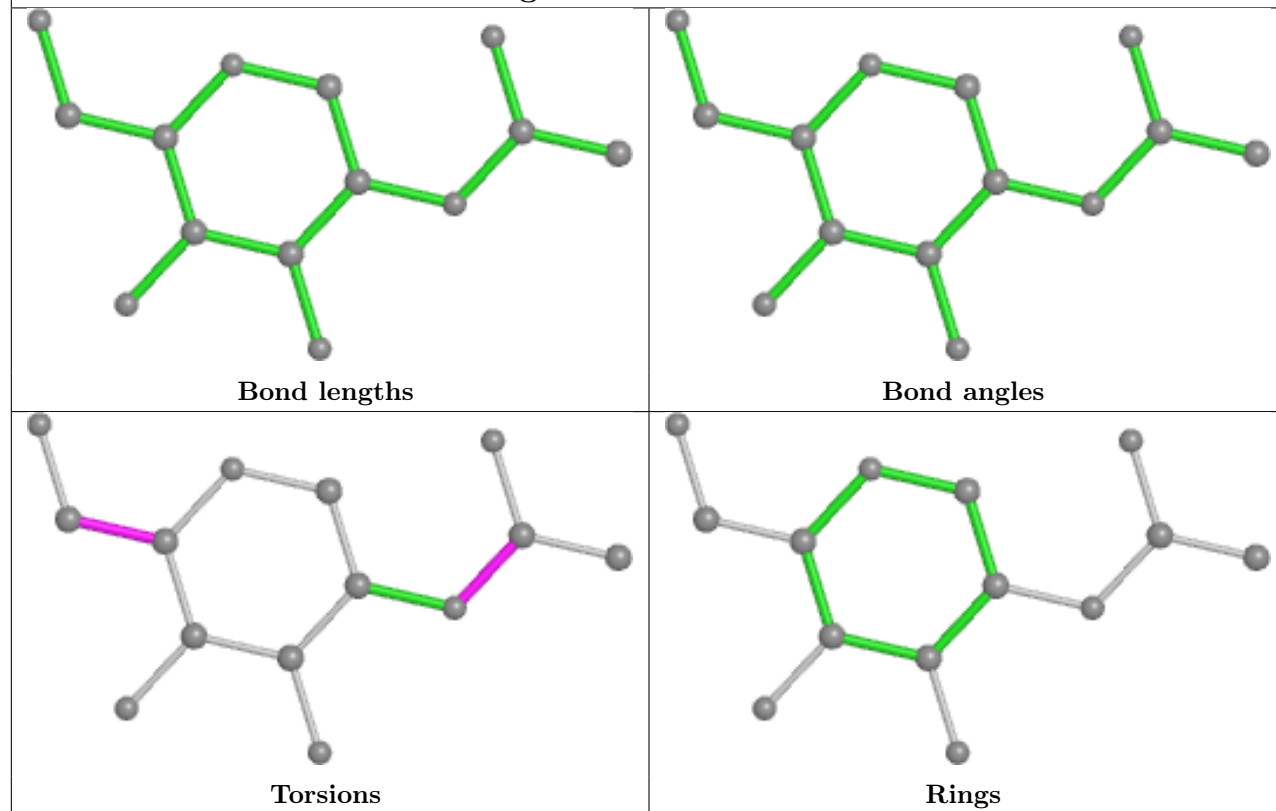




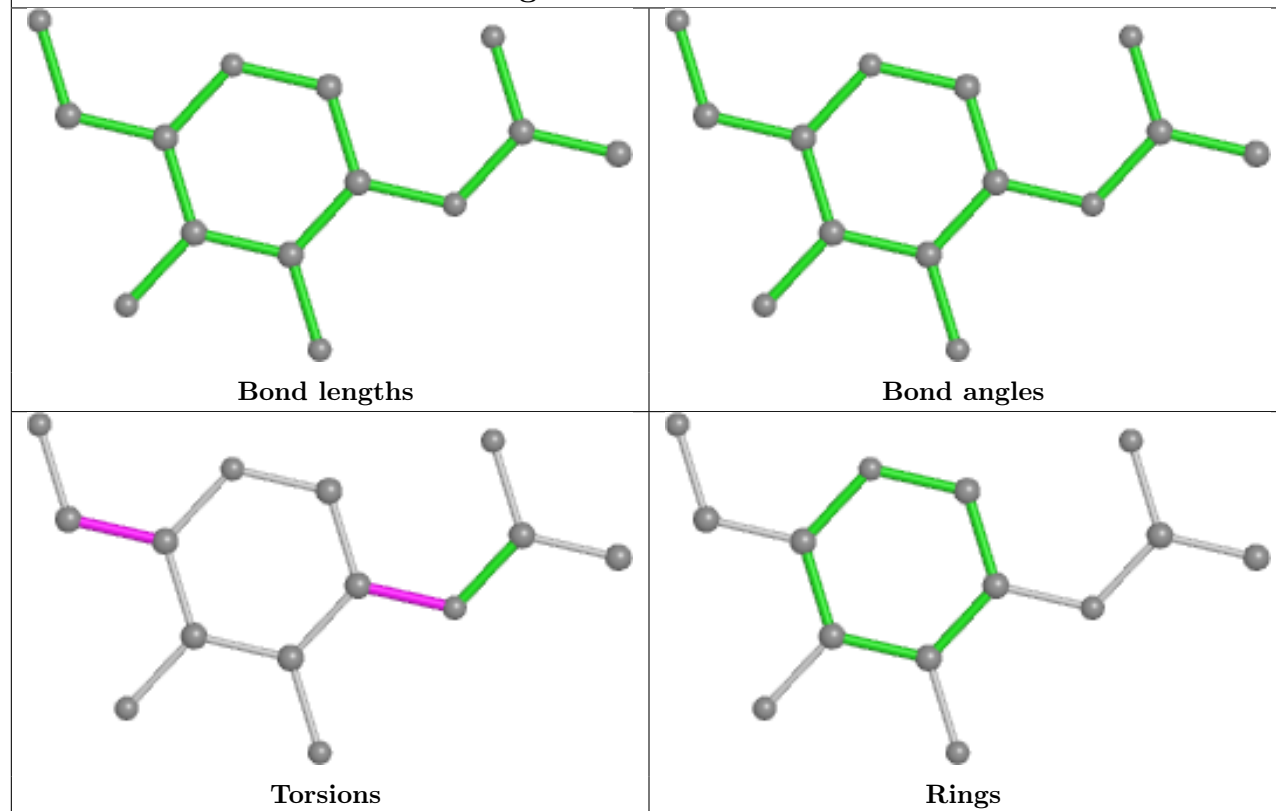
## Ligand NAG C 1202



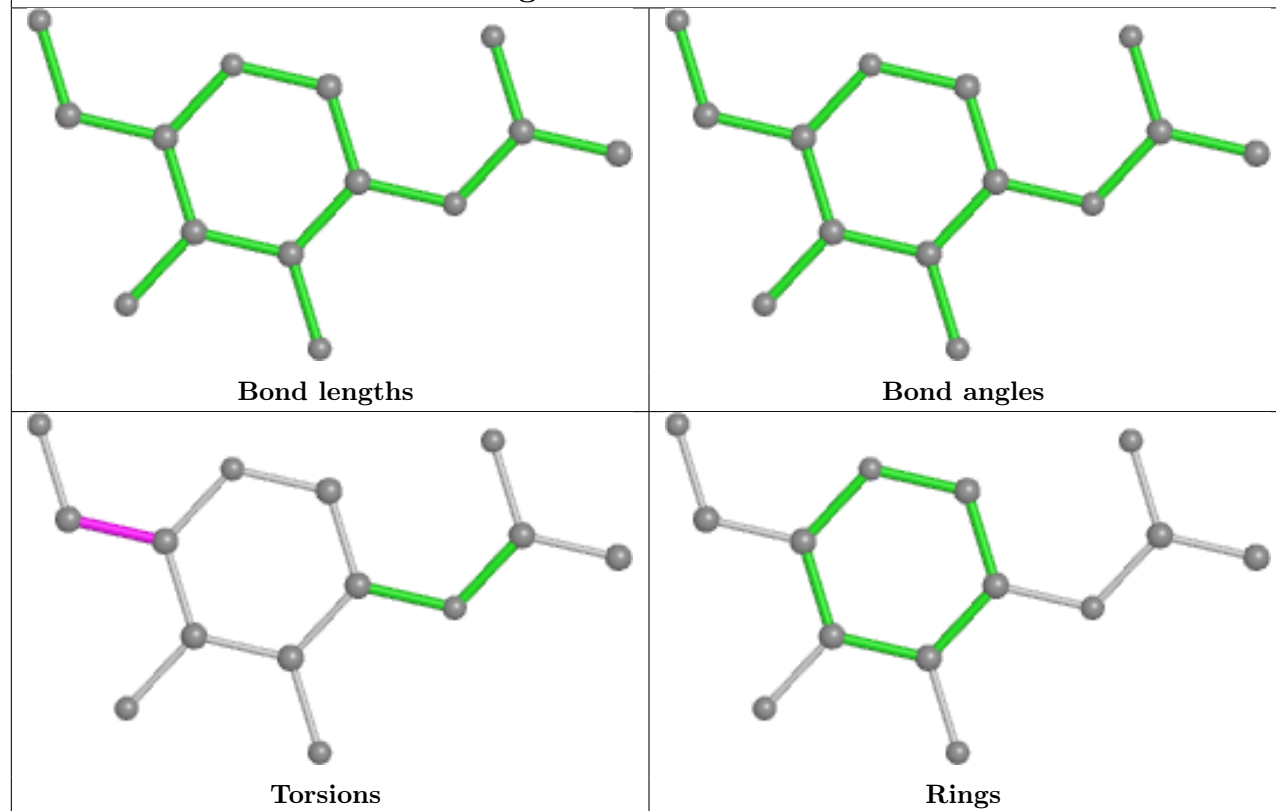
## Ligand NAG B 1202



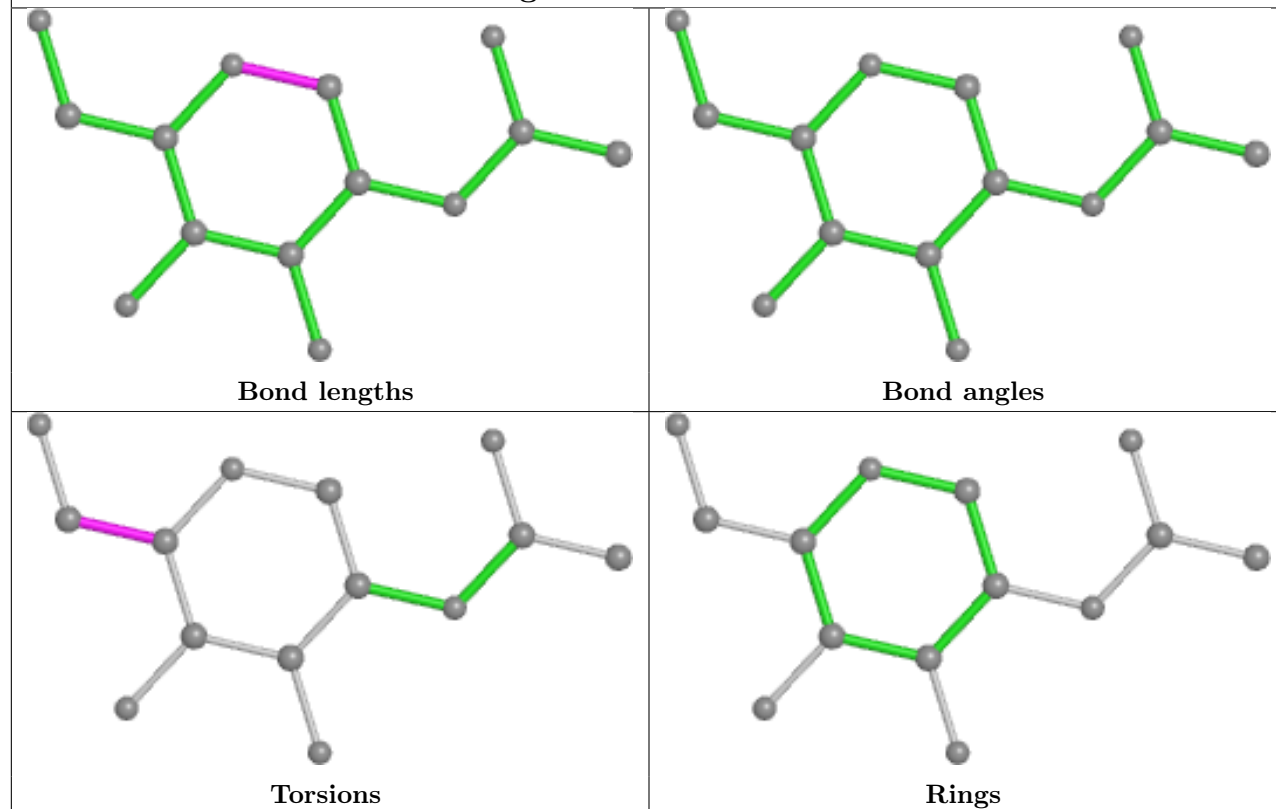
## Ligand NAG C 1208



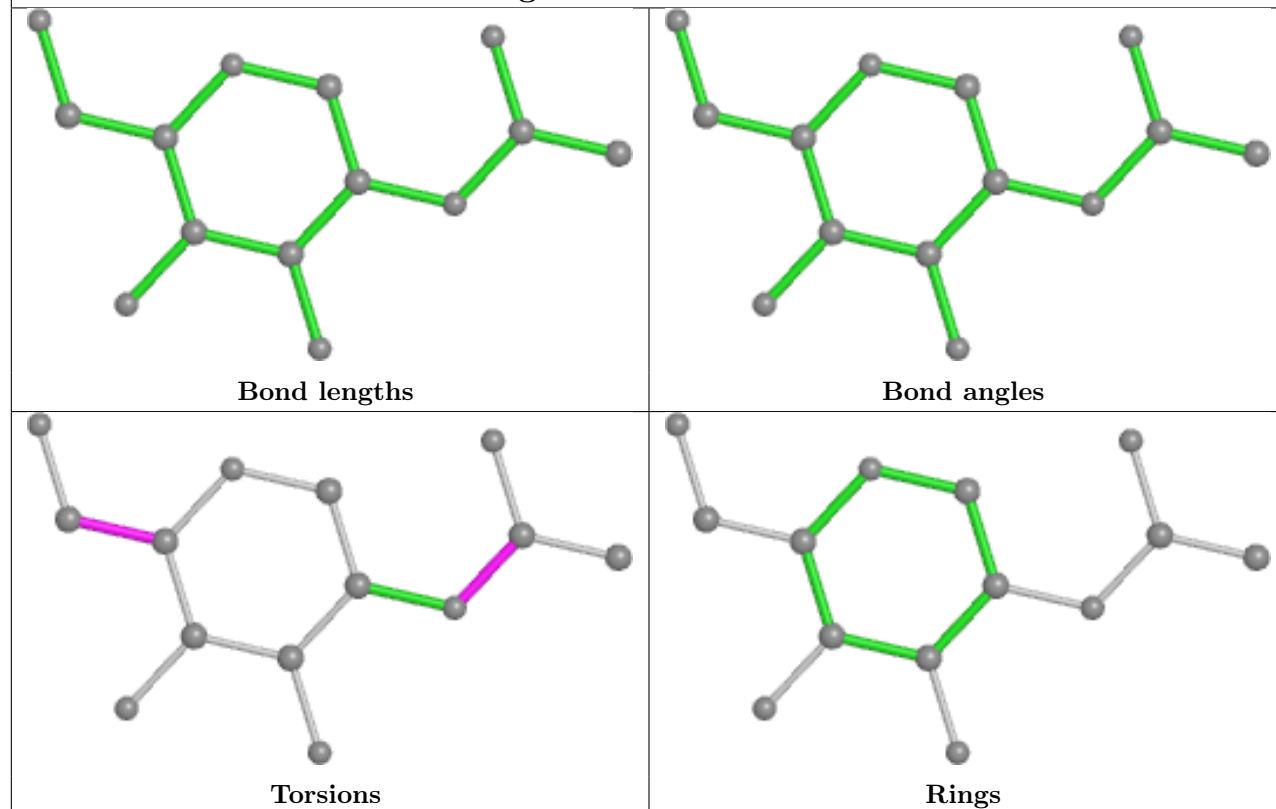
## Ligand NAG A 1210



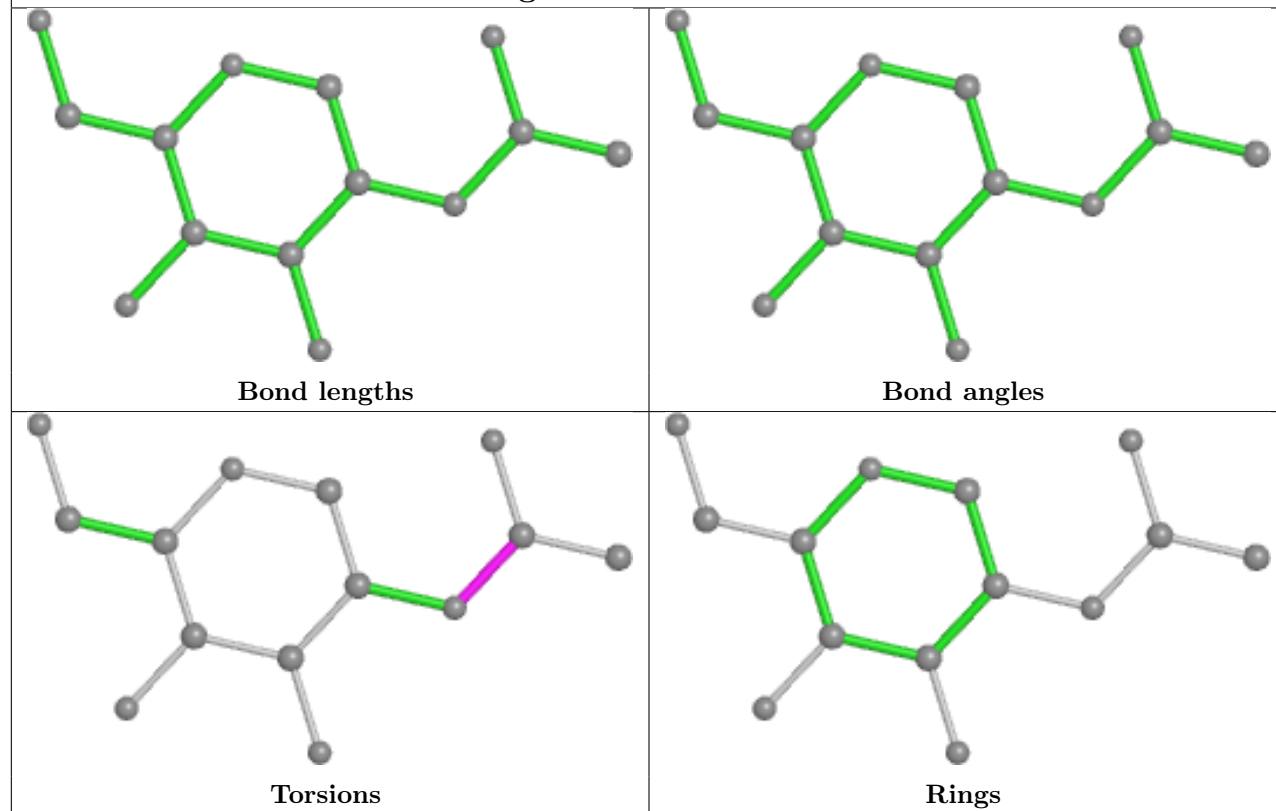
## Ligand NAG B 1209



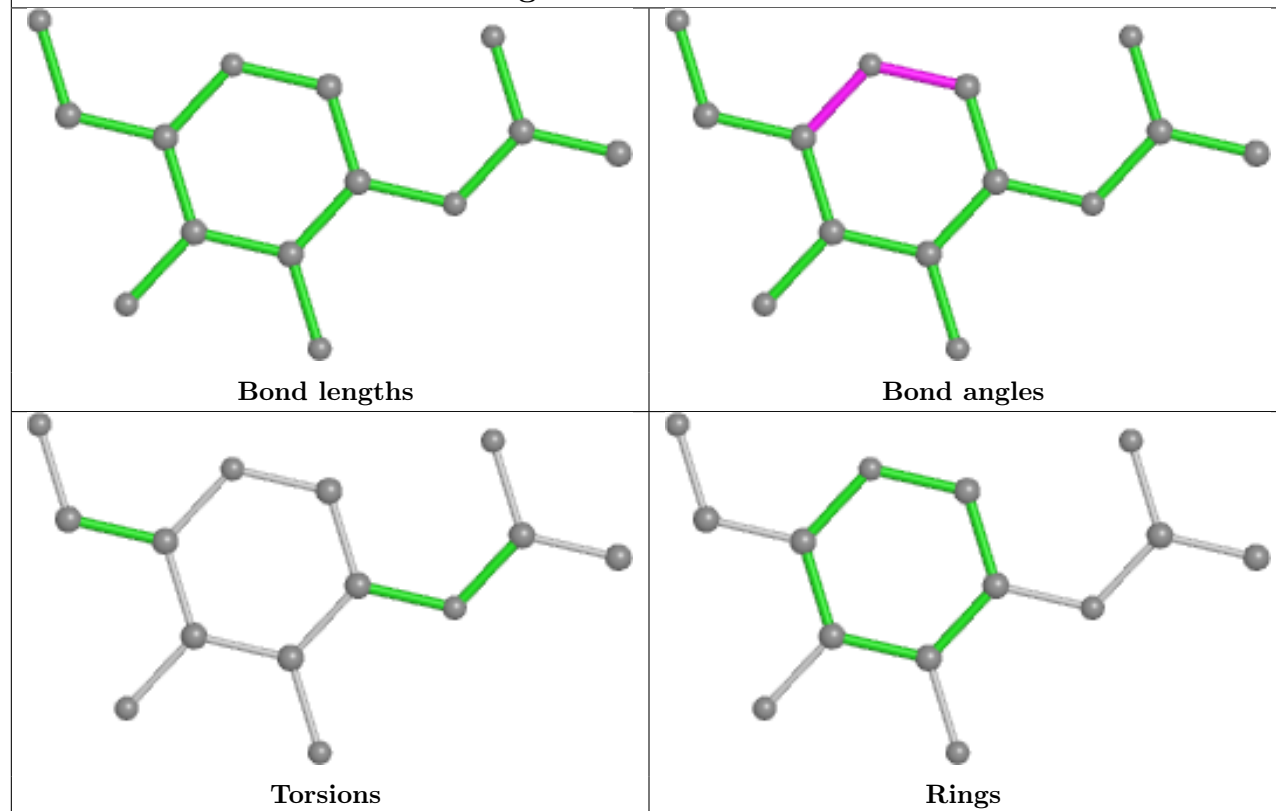
## Ligand NAG A 1202



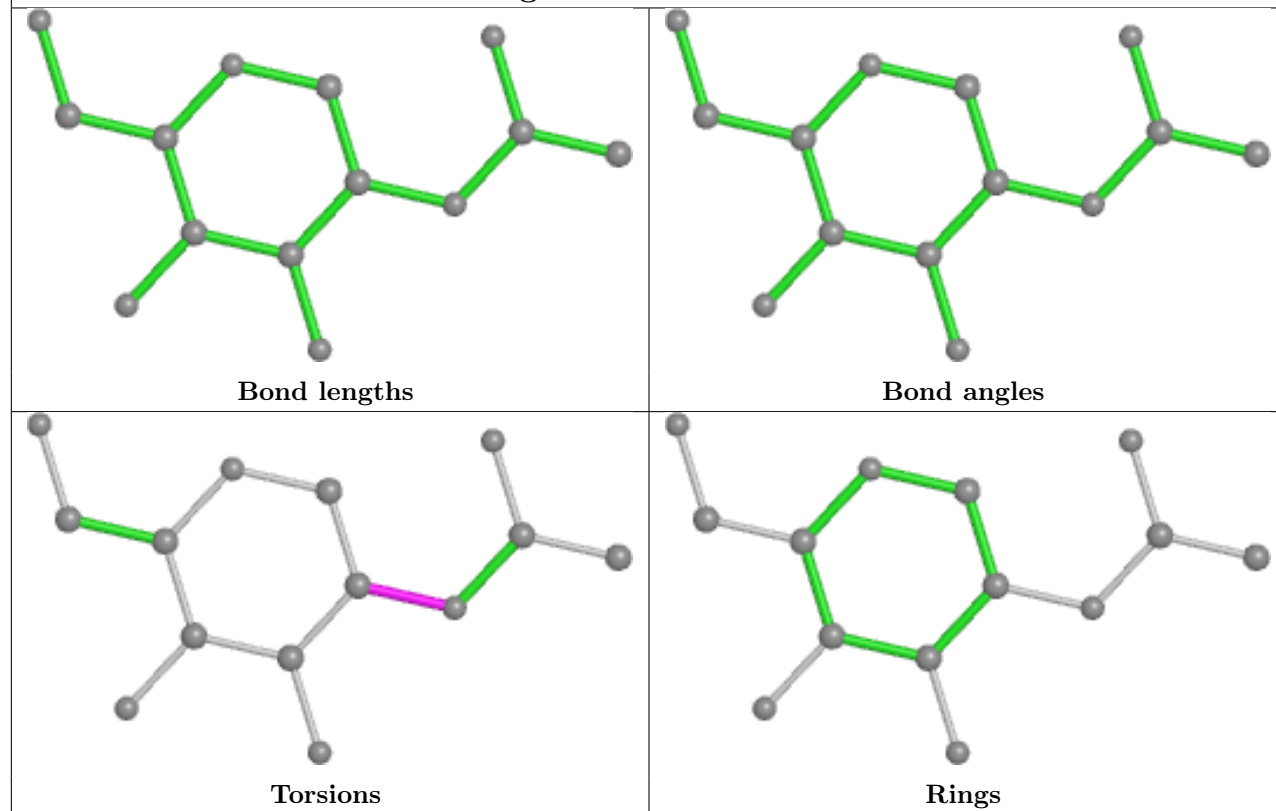
## Ligand NAG A 1203



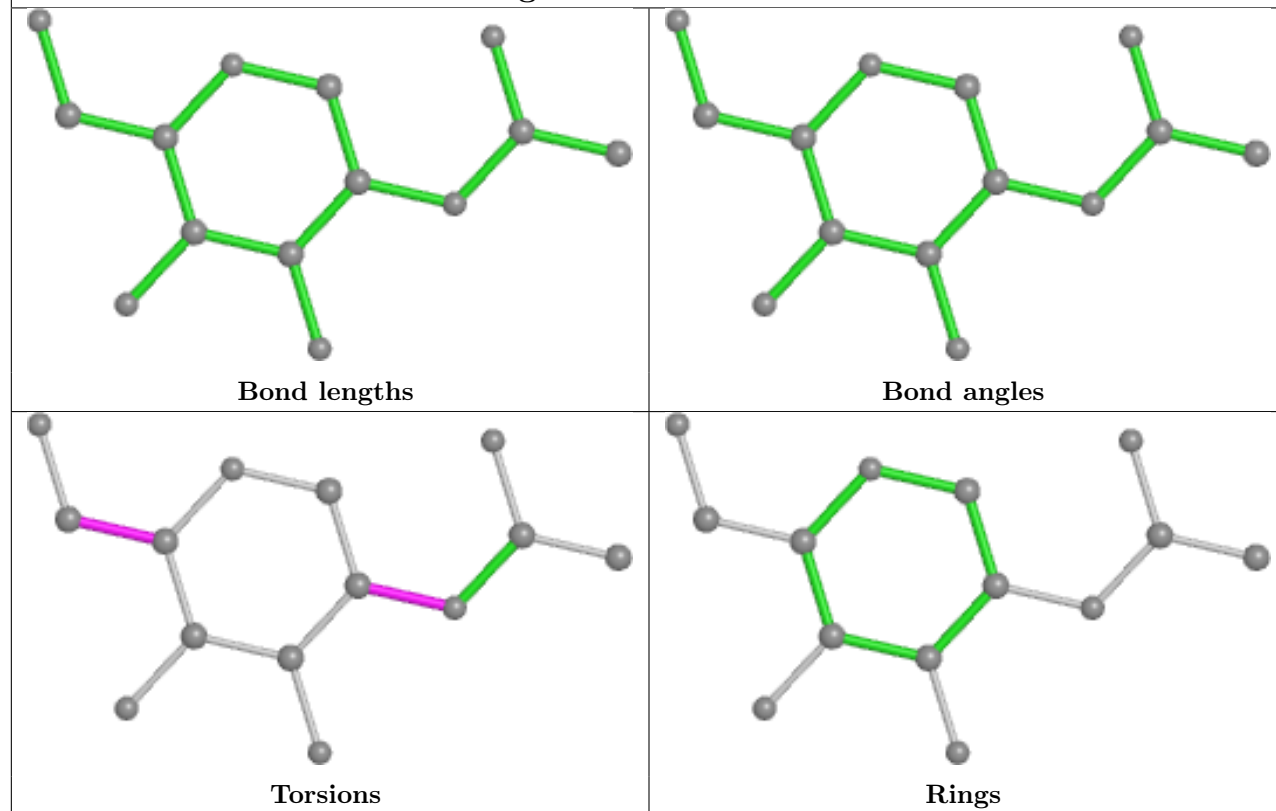
## Ligand NAG A 1207

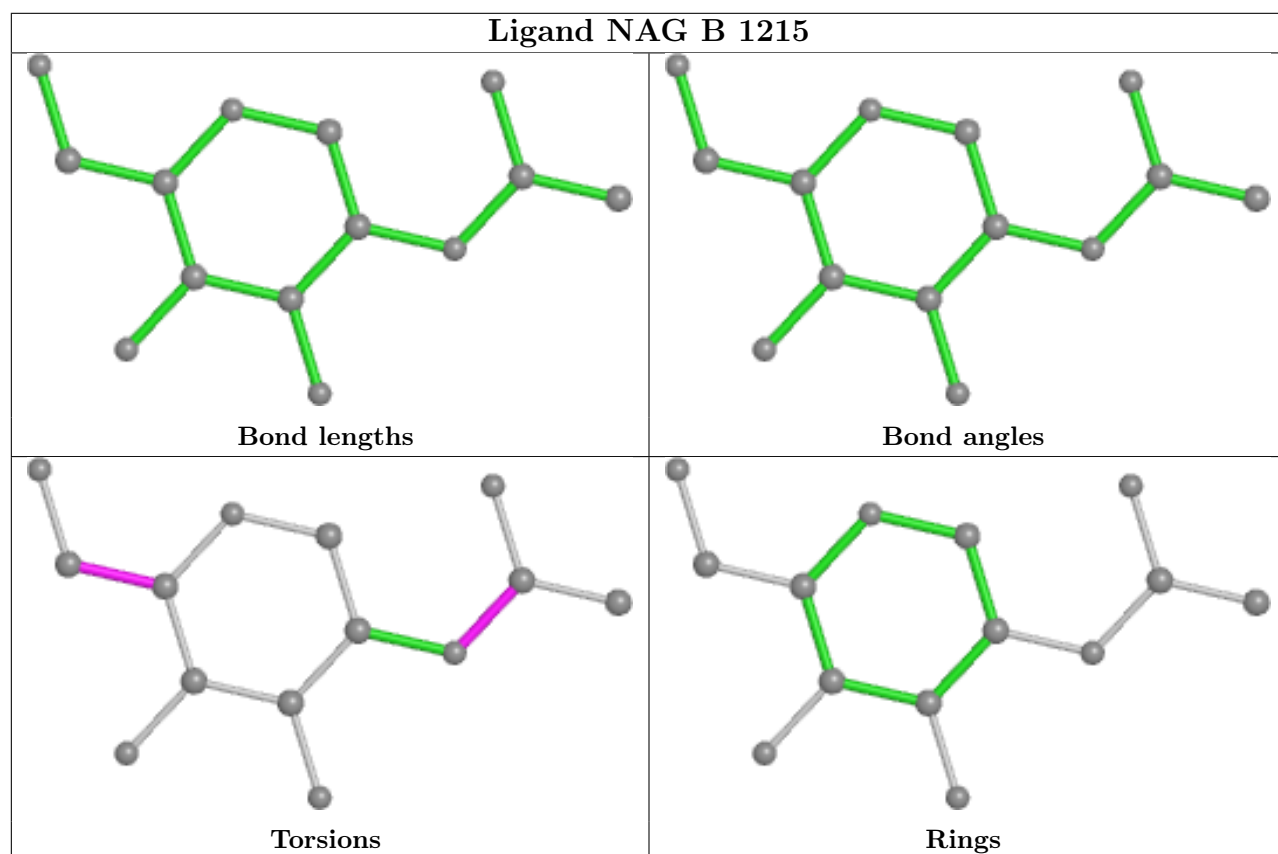
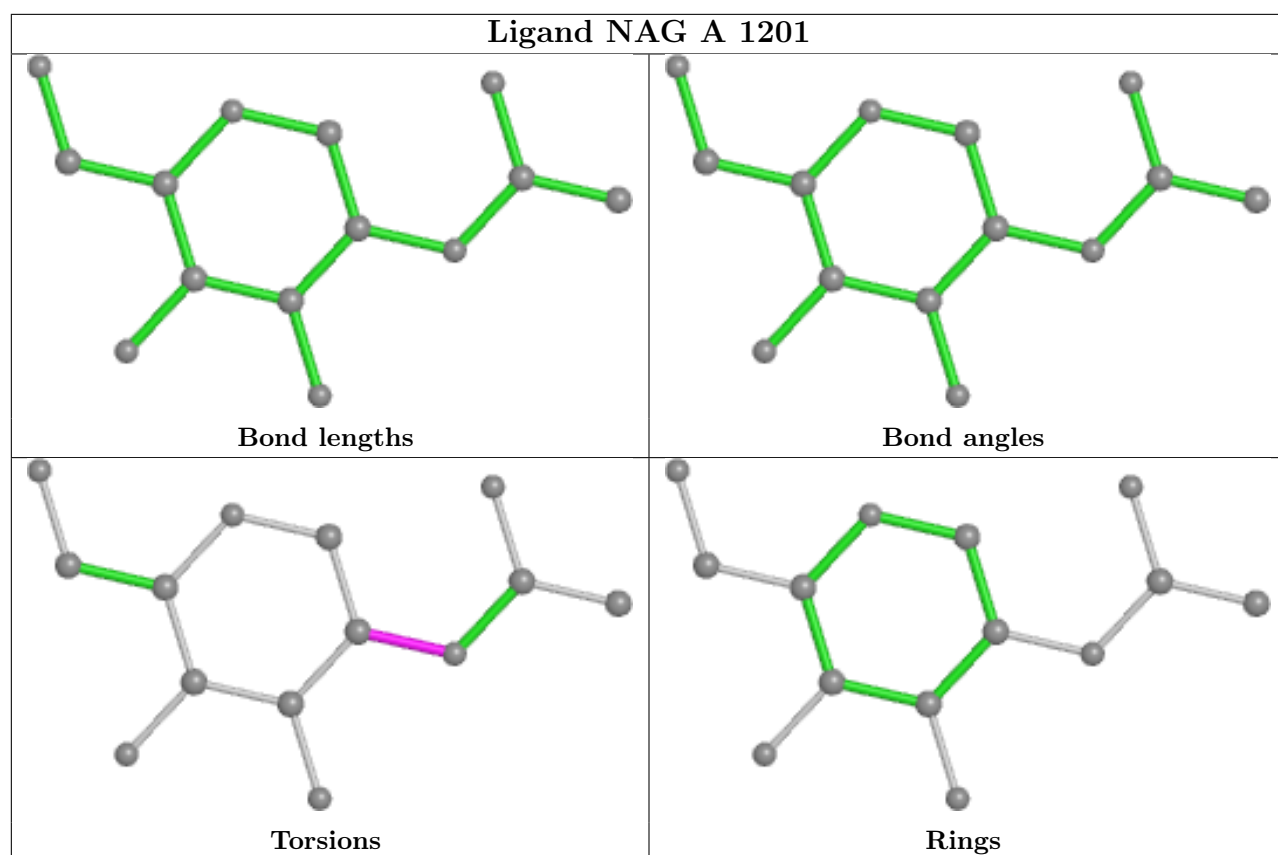


## Ligand NAG B 1201

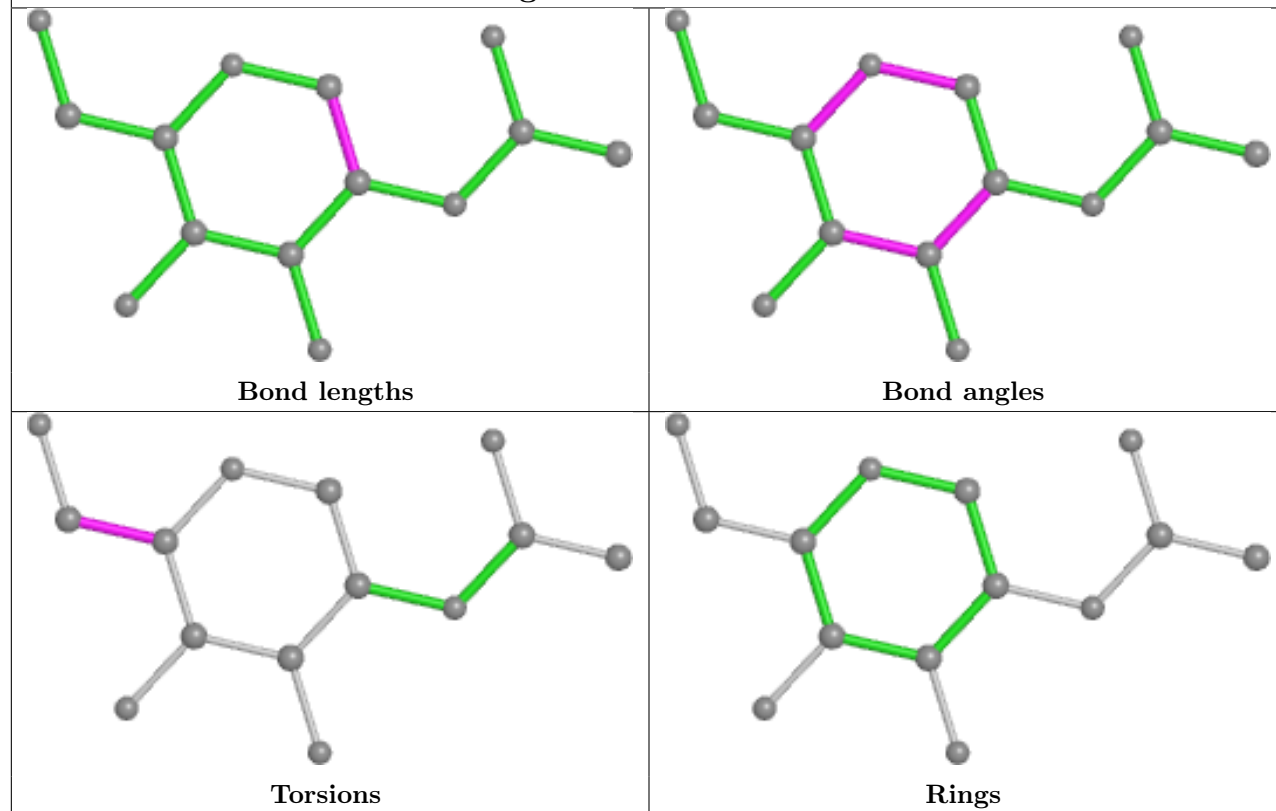


## Ligand NAG A 1208

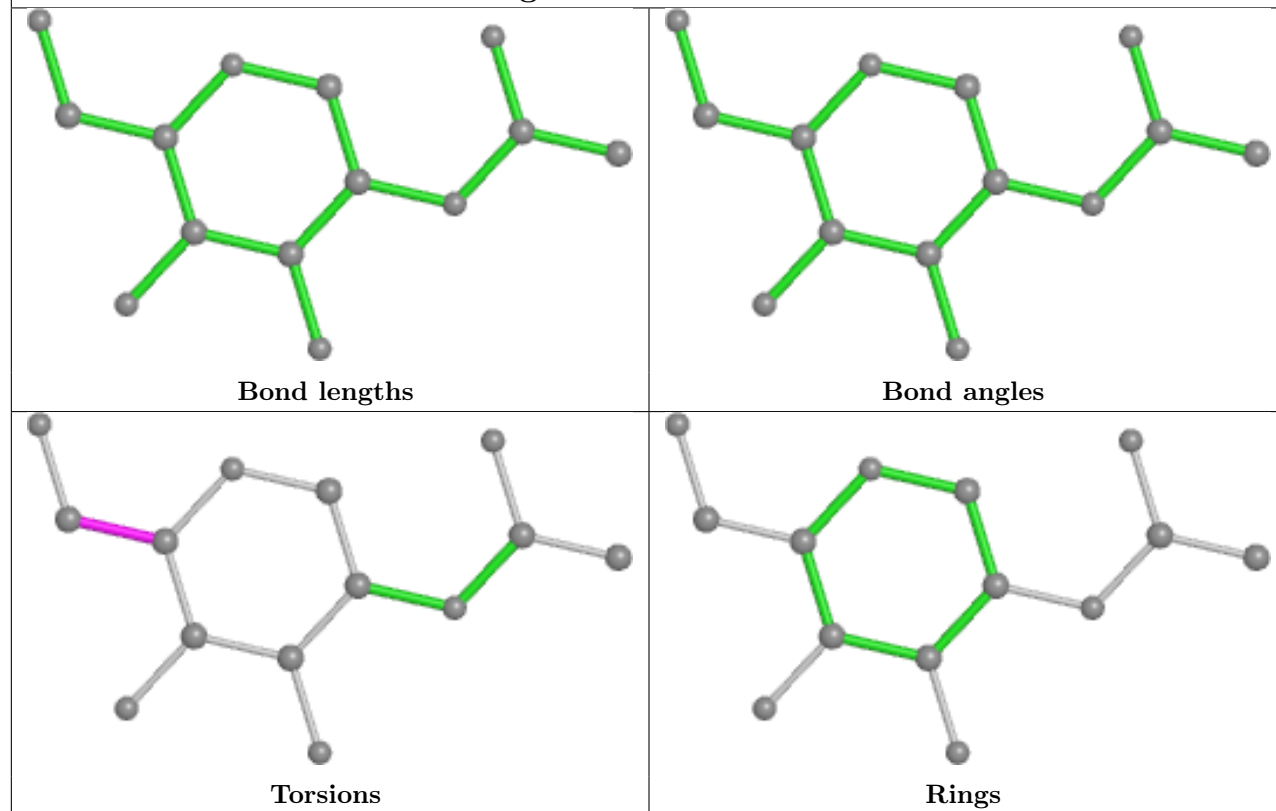




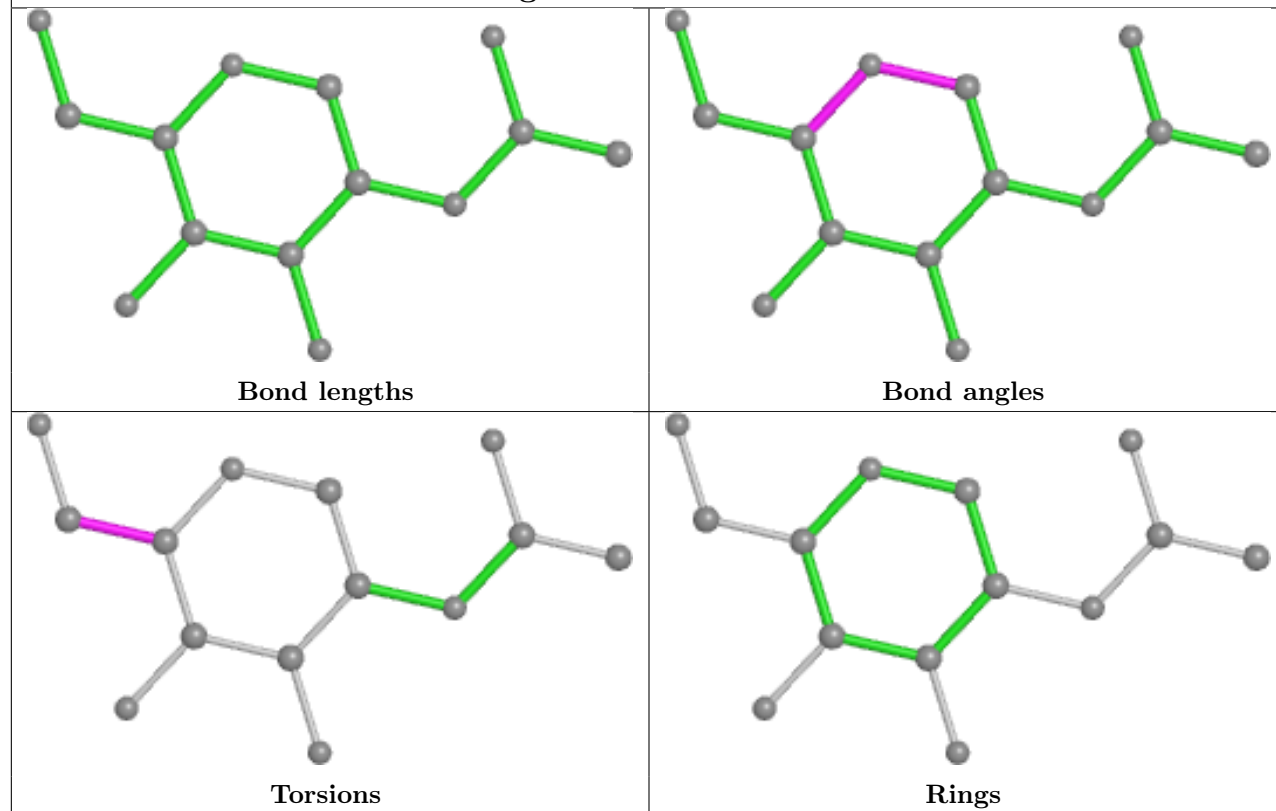
## Ligand NAG C 1211



## Ligand NAG B 1210



## Ligand NAG C 1214

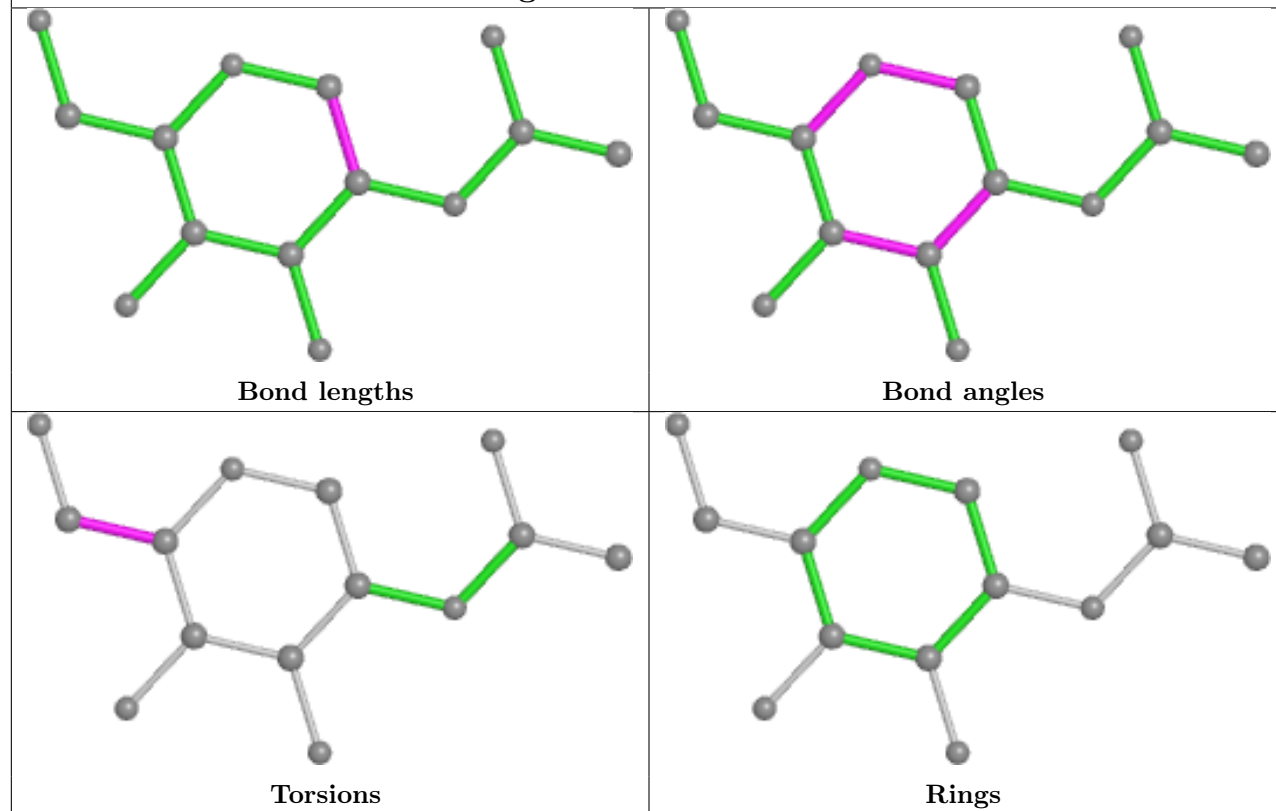


## Ligand NAG A 1212

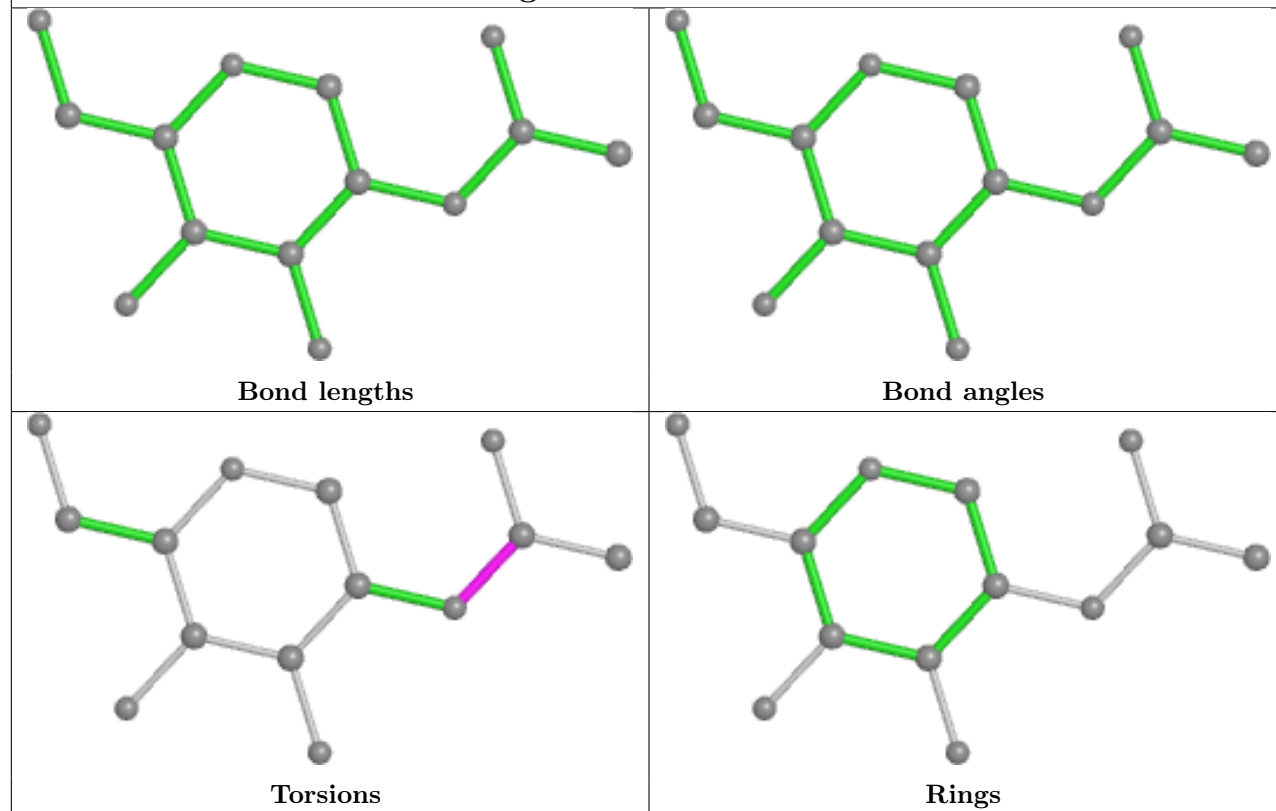




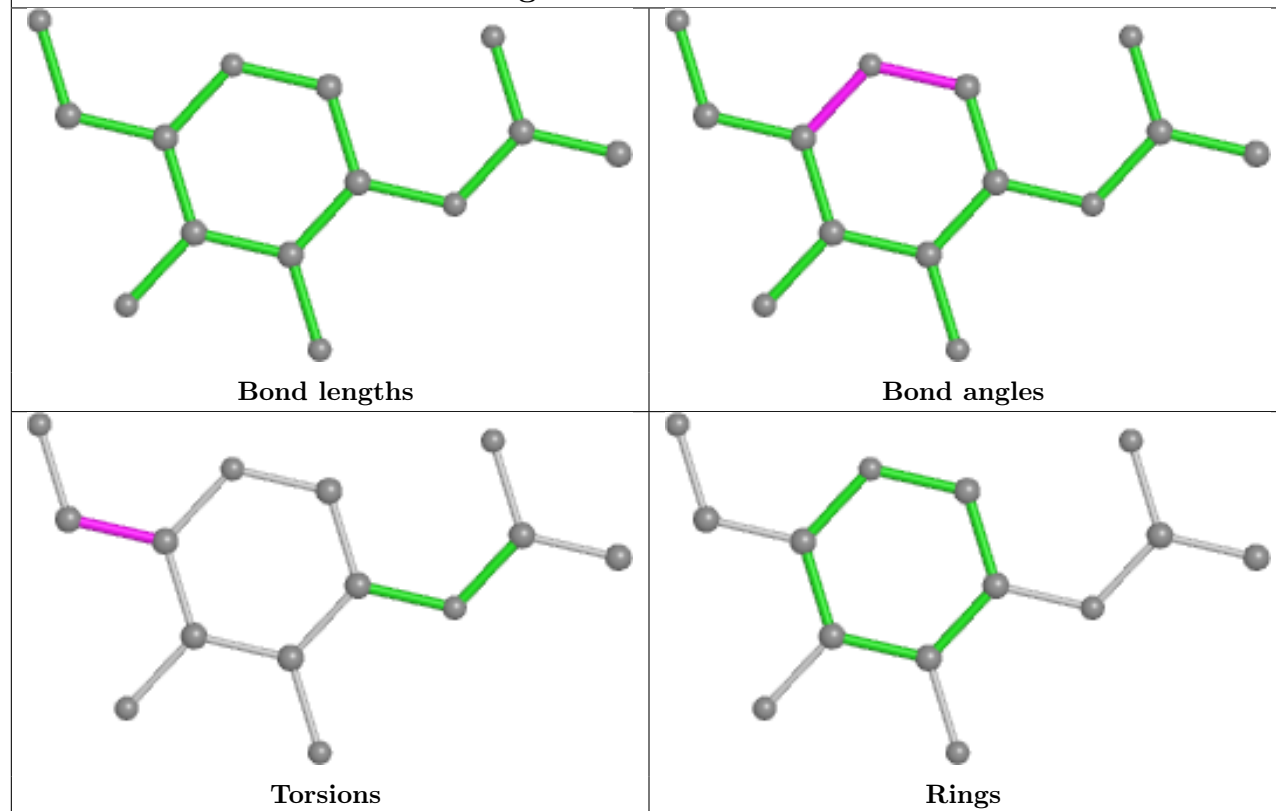
## Ligand NAG A 1211



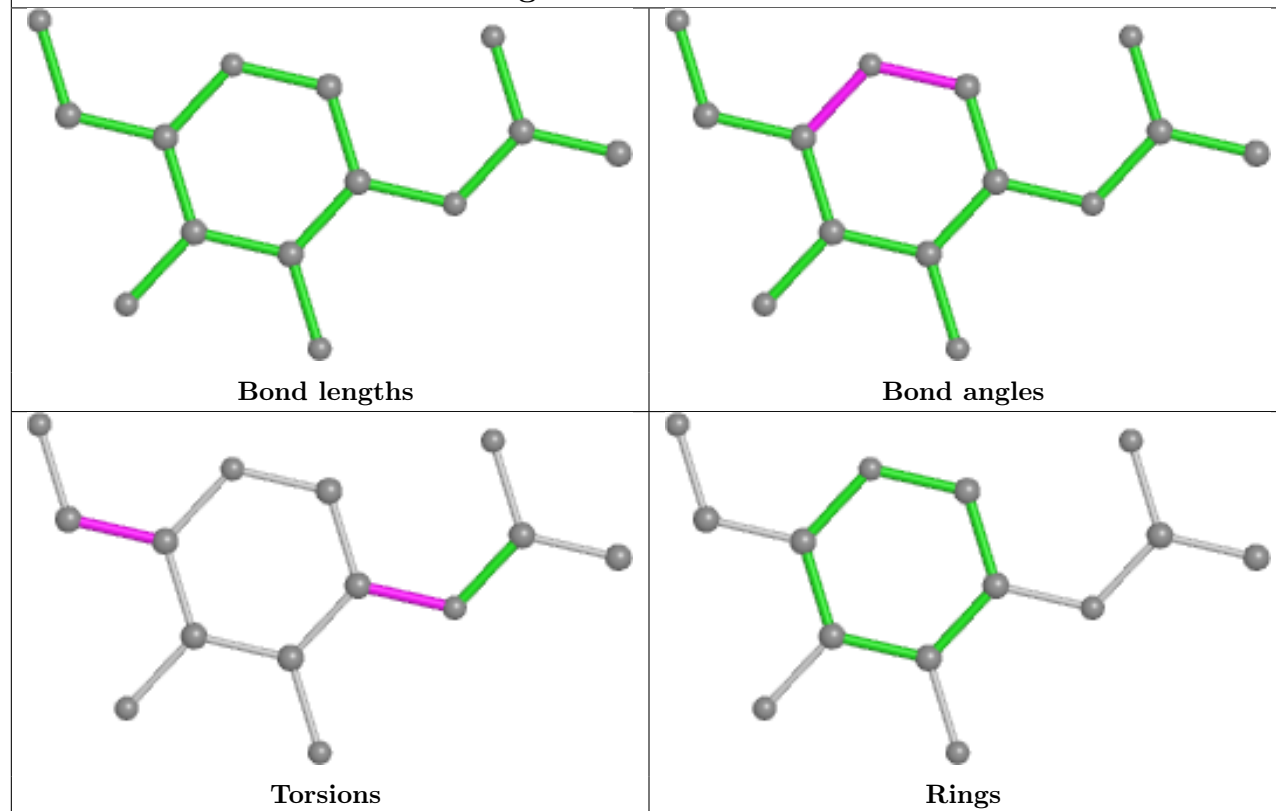
## Ligand NAG C 1203



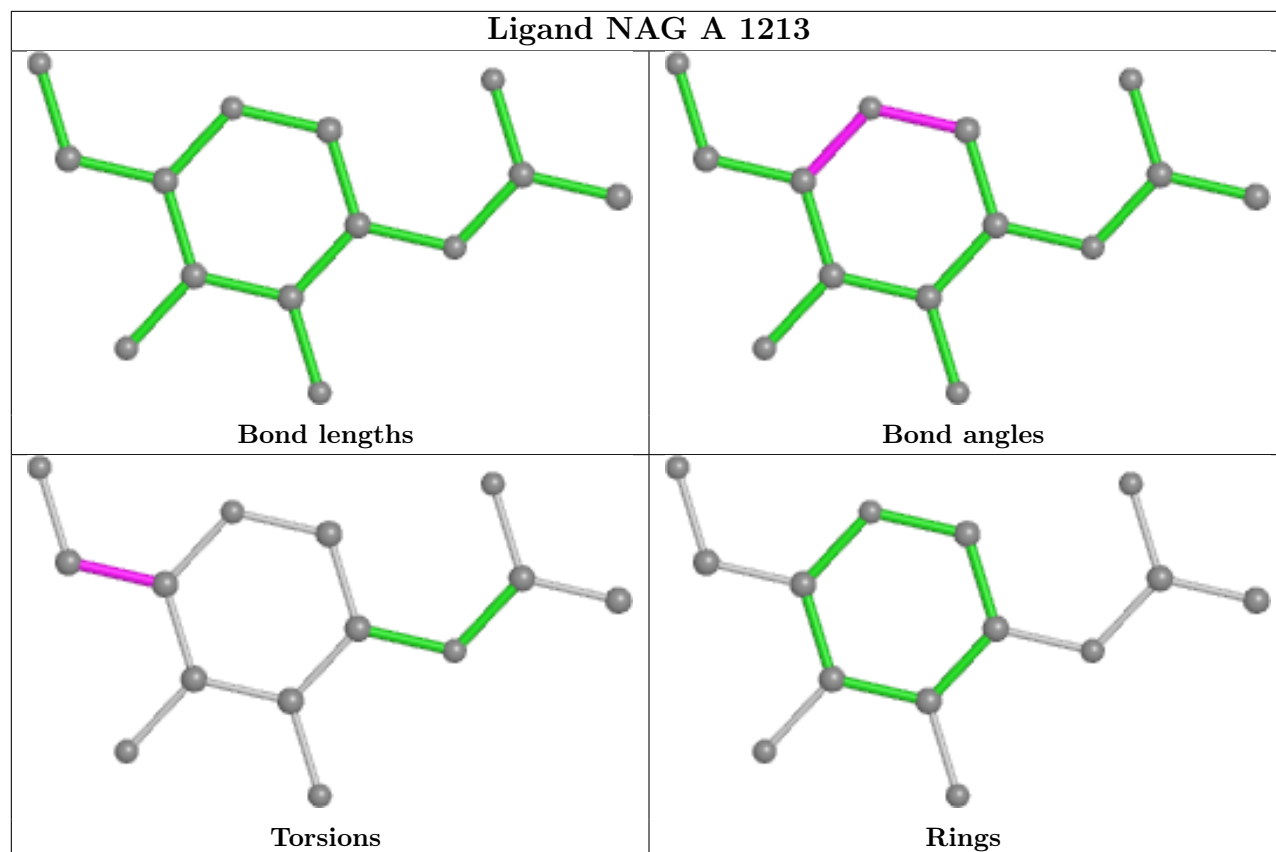
## Ligand NAG A 1214



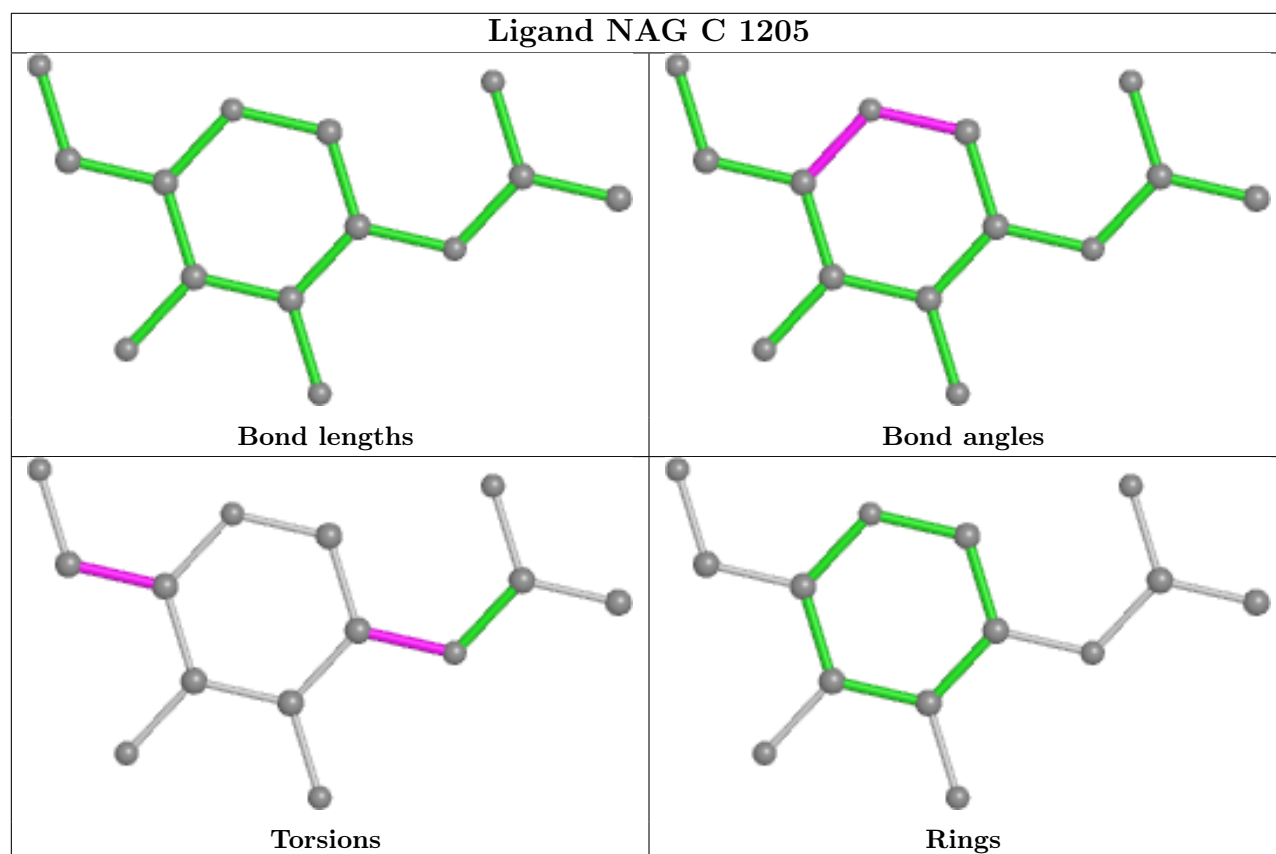
## Ligand NAG A 1205



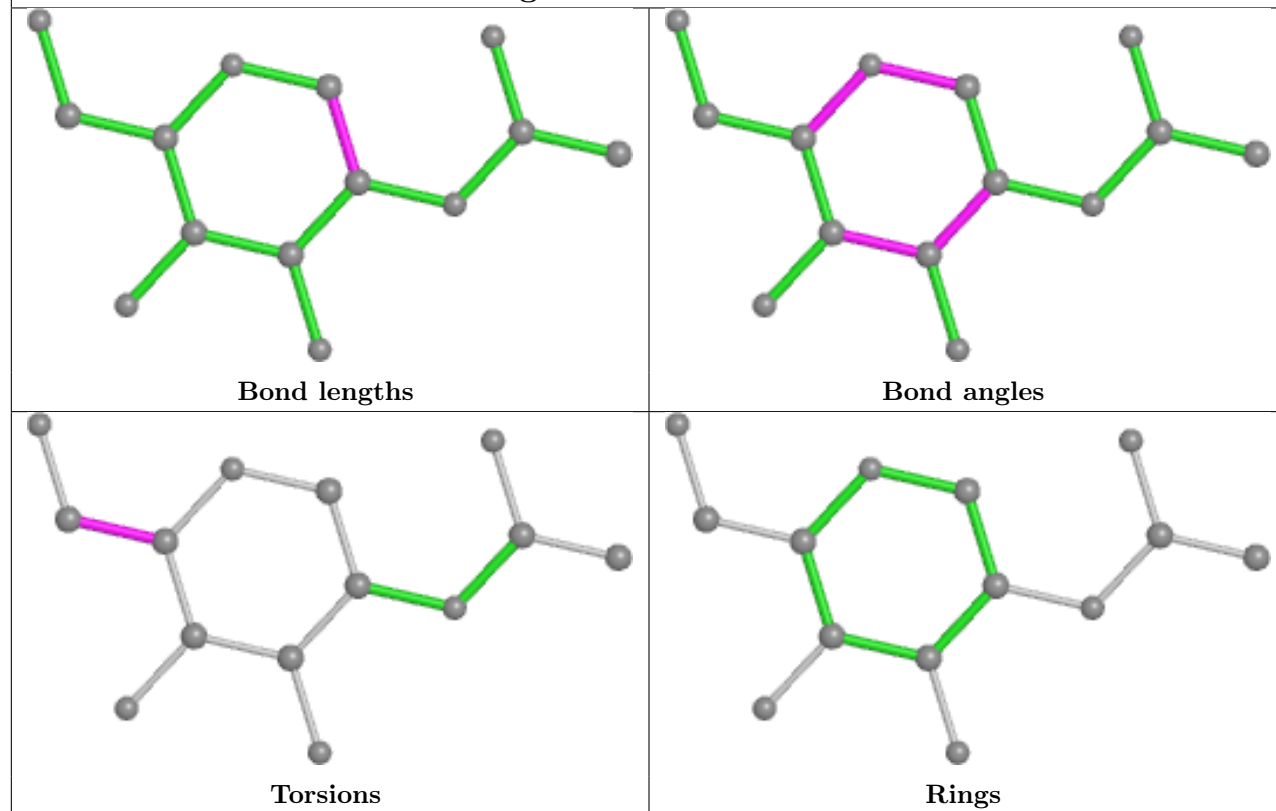
## Ligand NAG A 1213



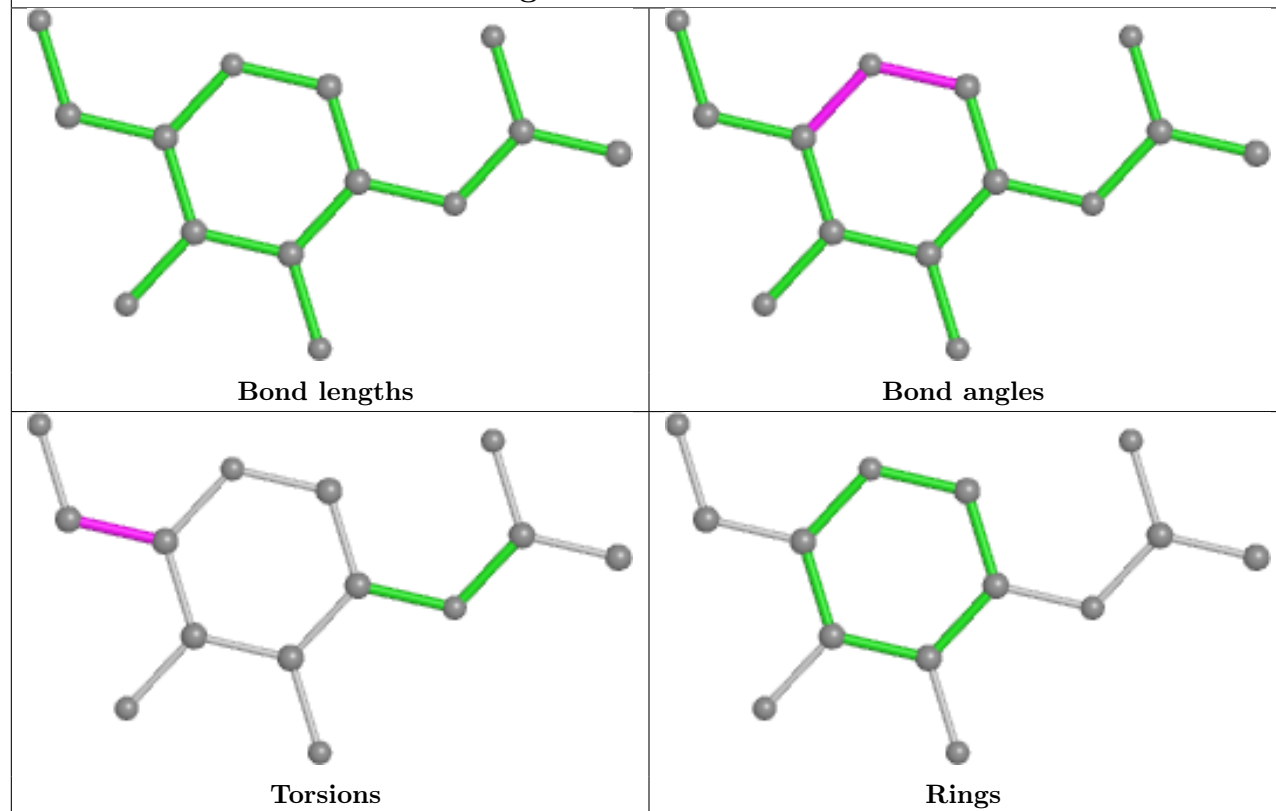
## Ligand NAG C 1205



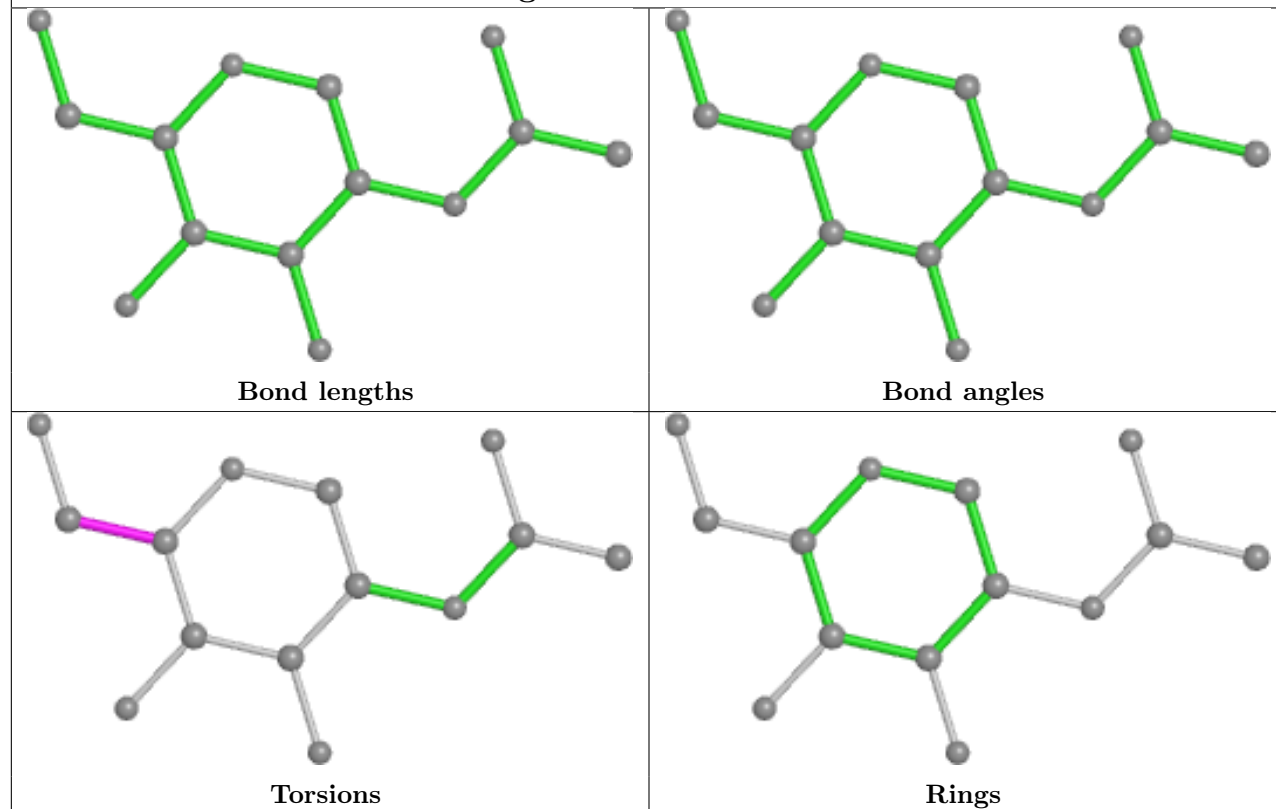
## Ligand NAG B 1211



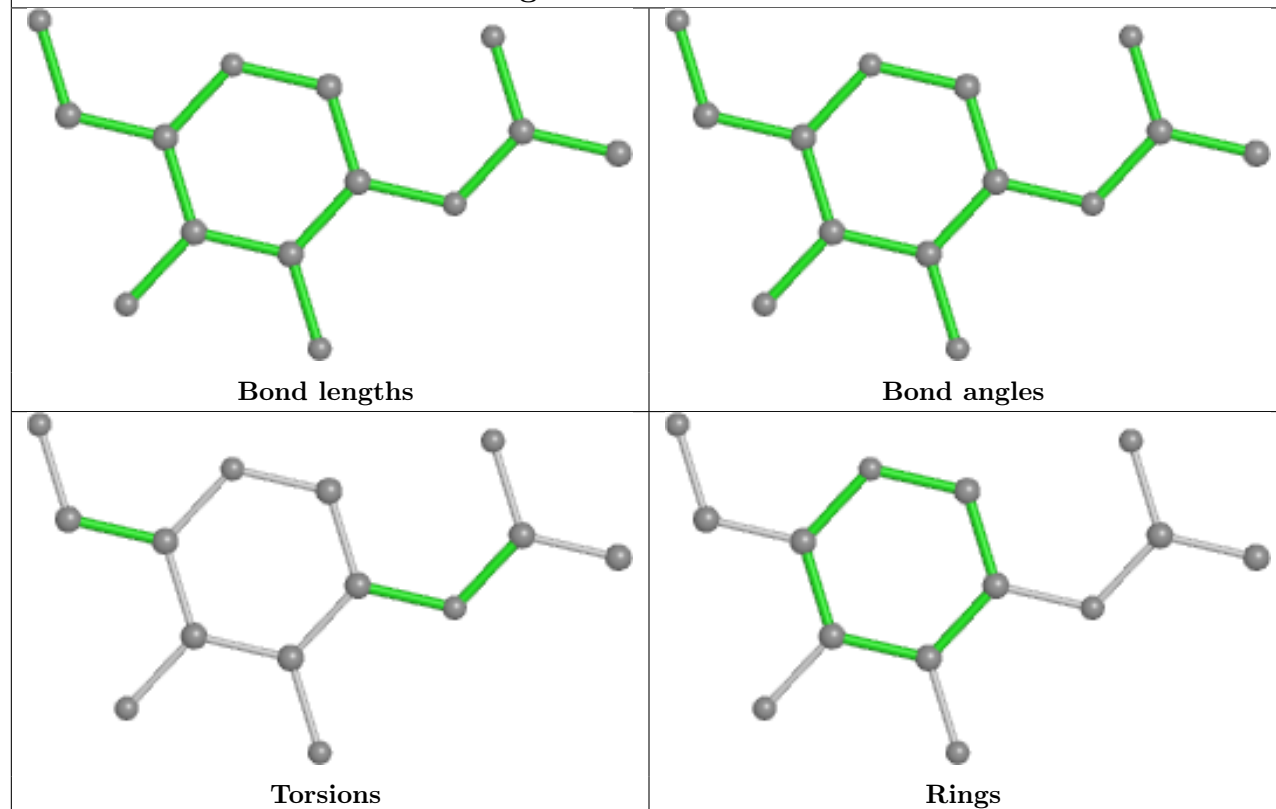
## Ligand NAG B 1214

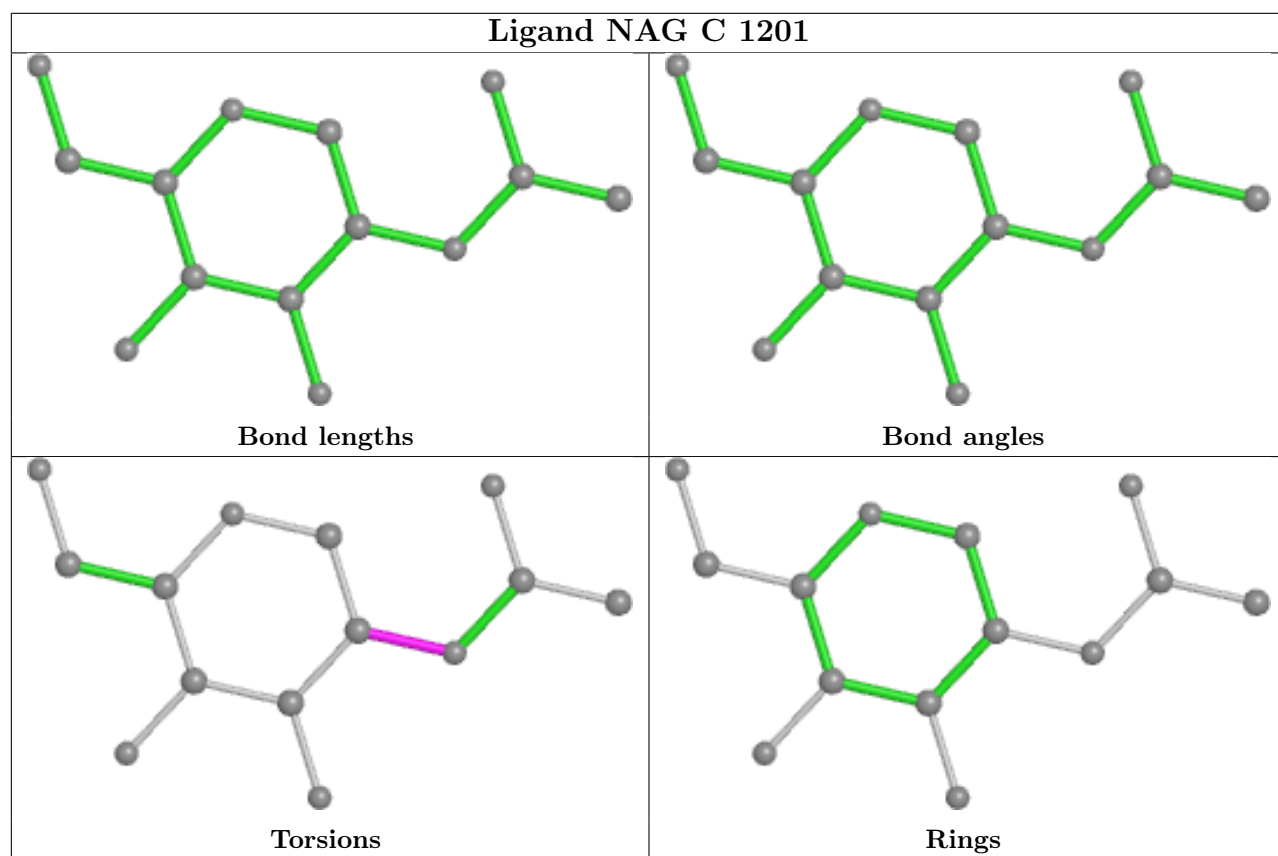
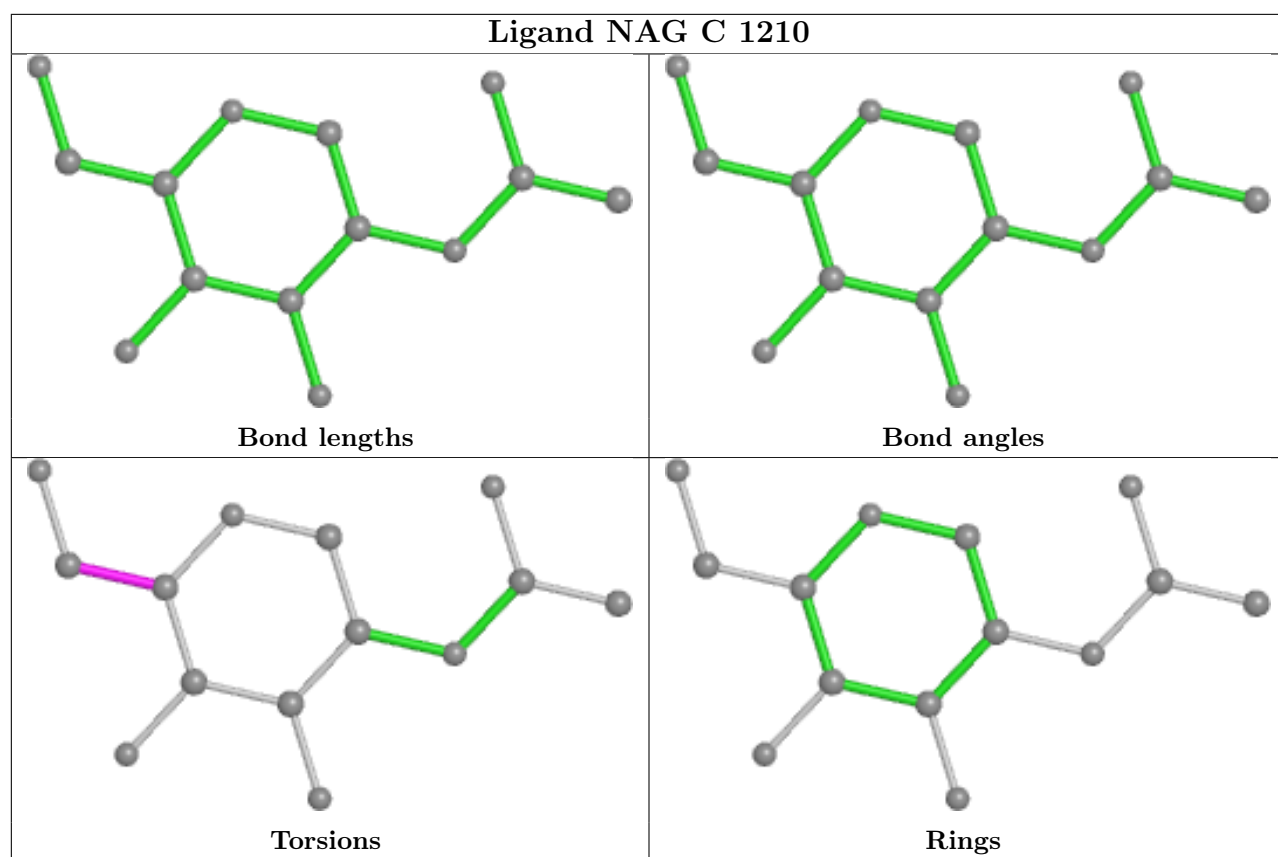


## Ligand NAG A 1206

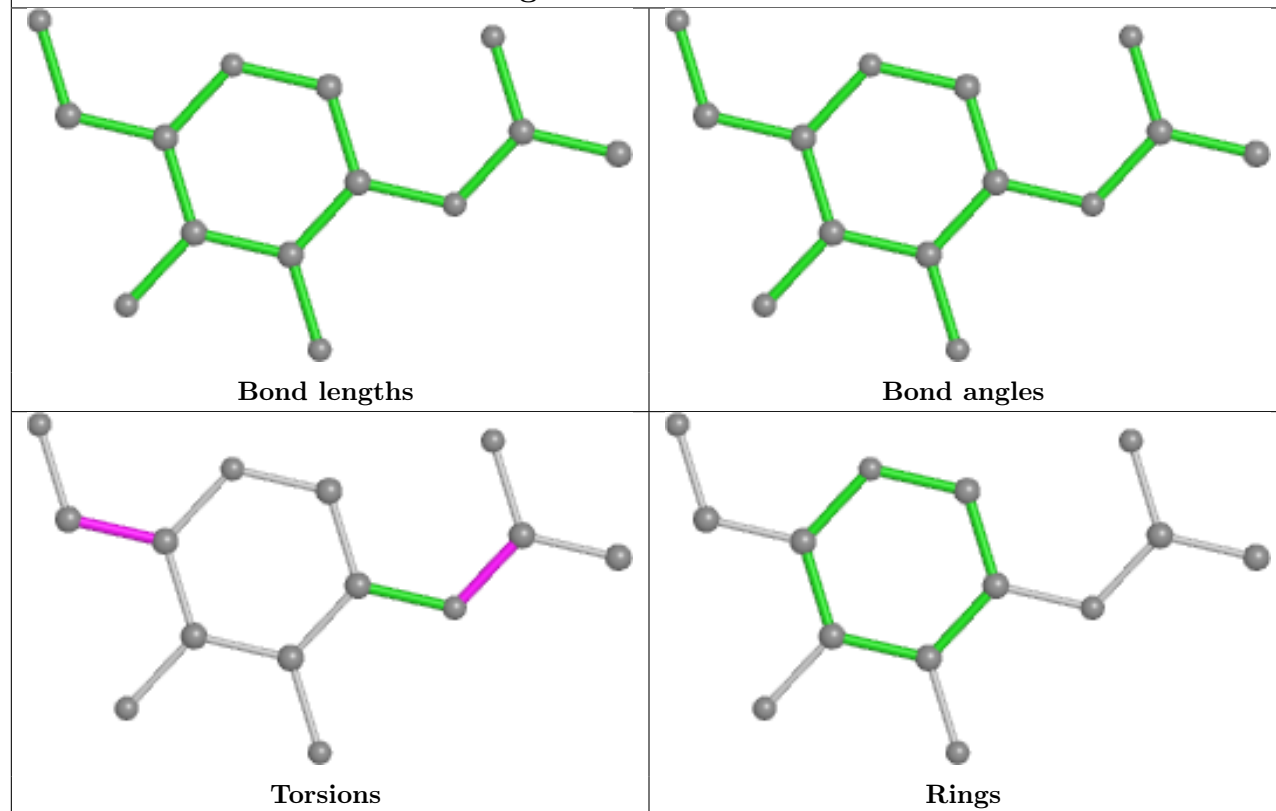


## Ligand NAG B 1204

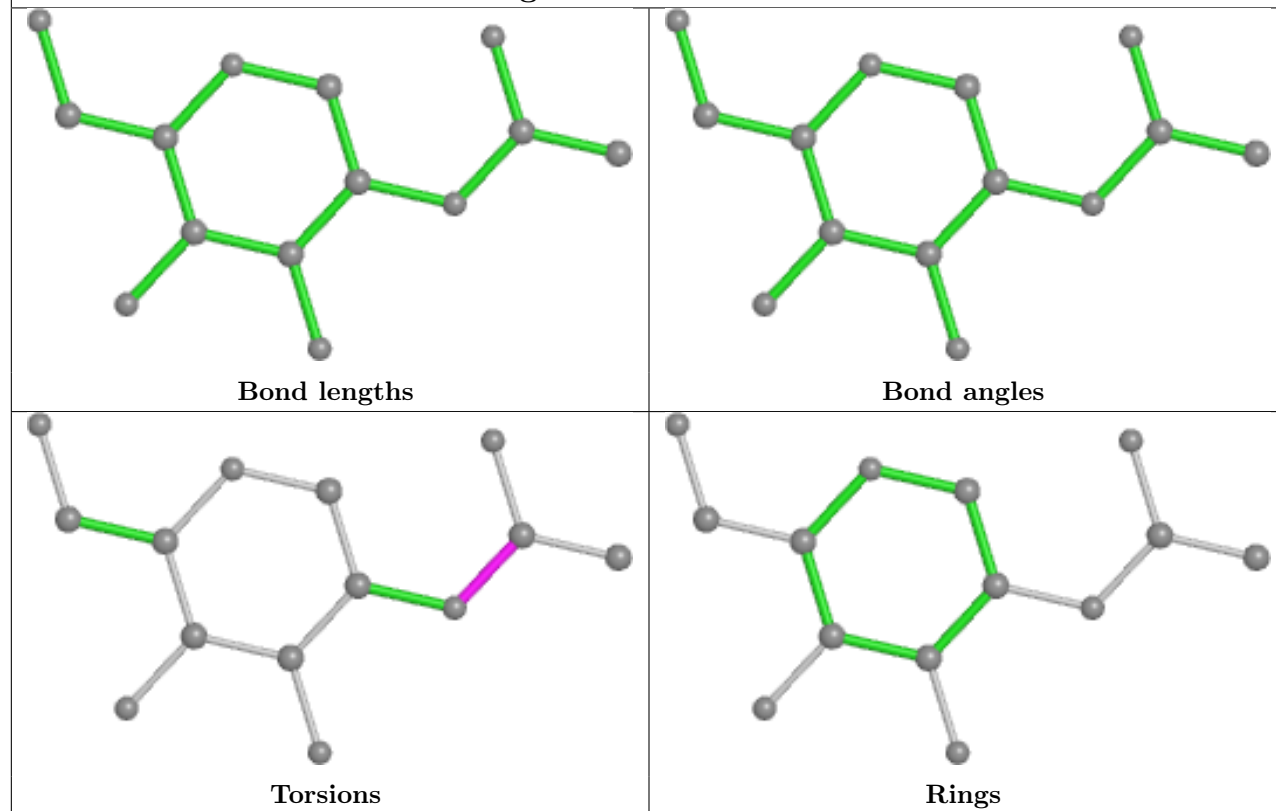




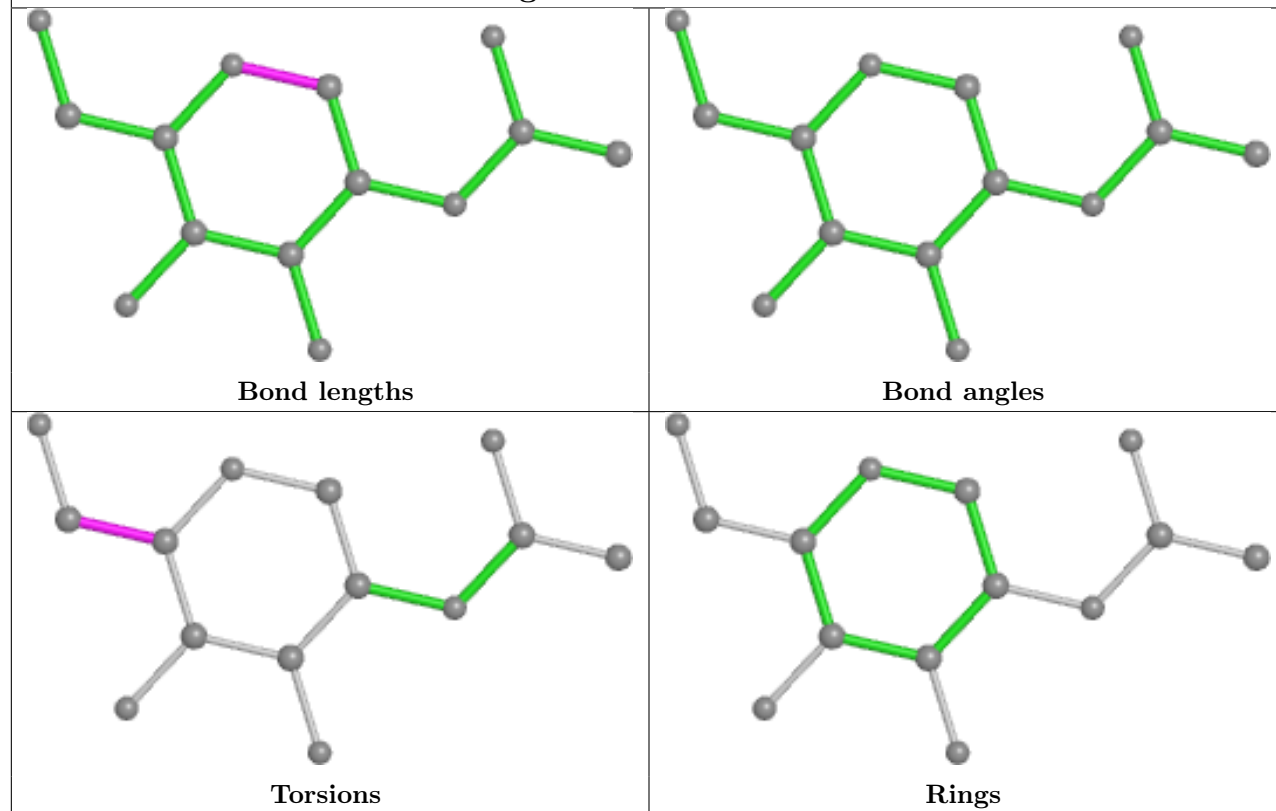
## Ligand NAG B 1216



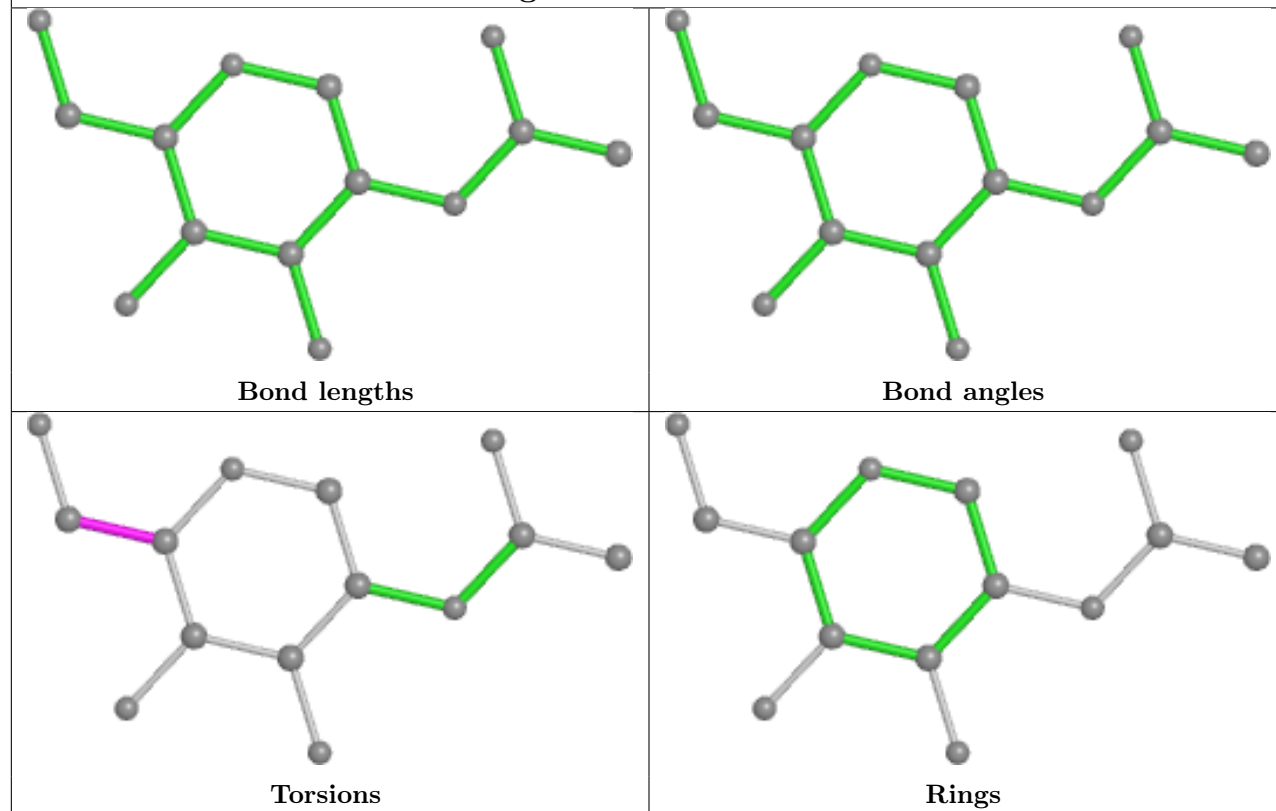
## Ligand NAG B 1203



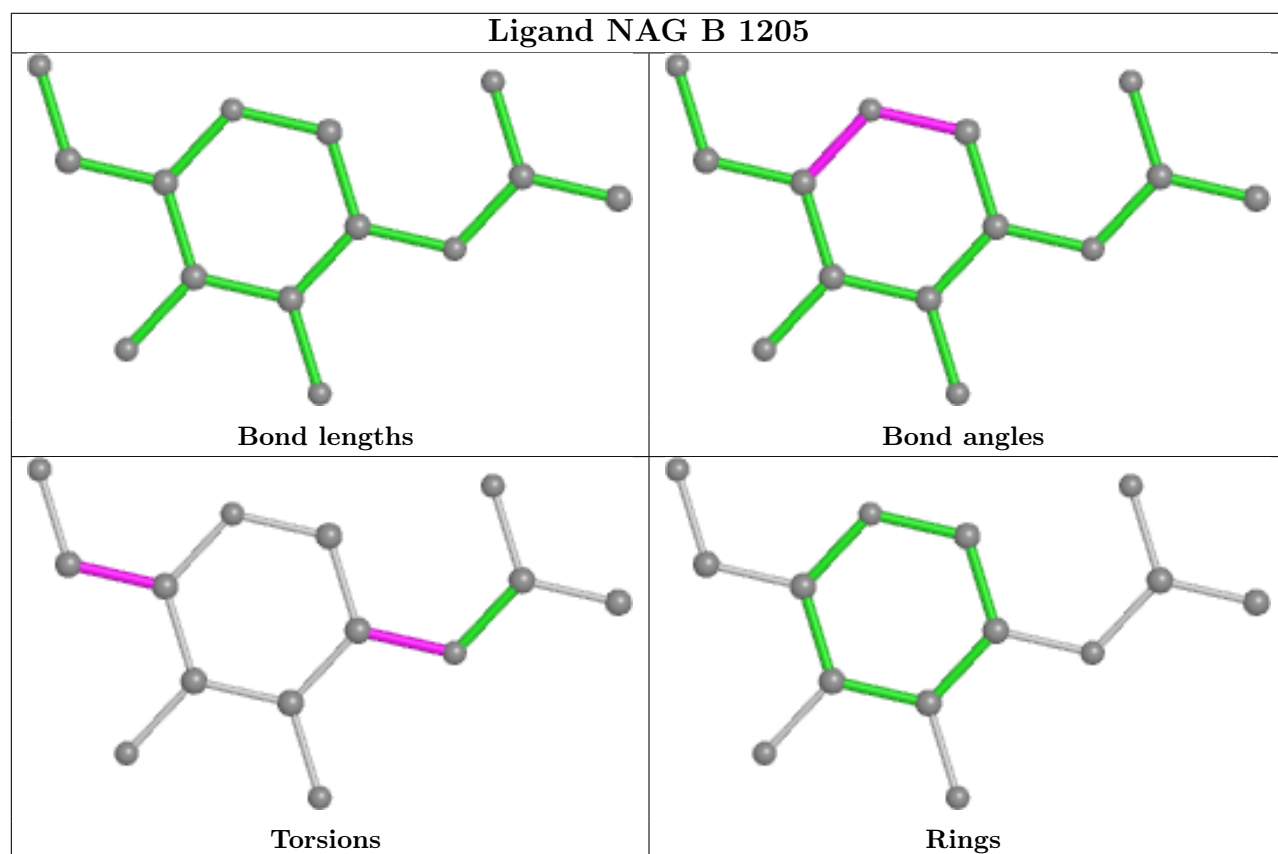
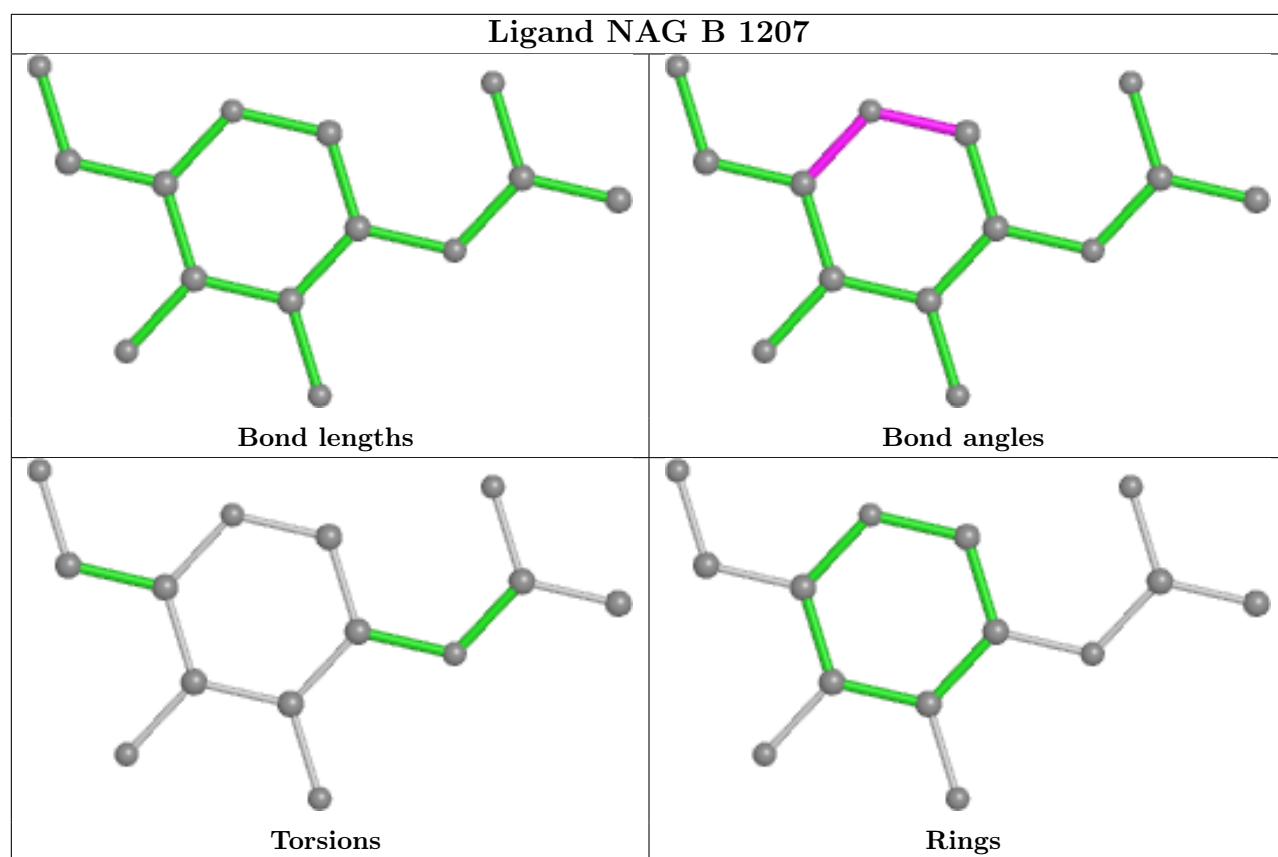
## Ligand NAG C 1209



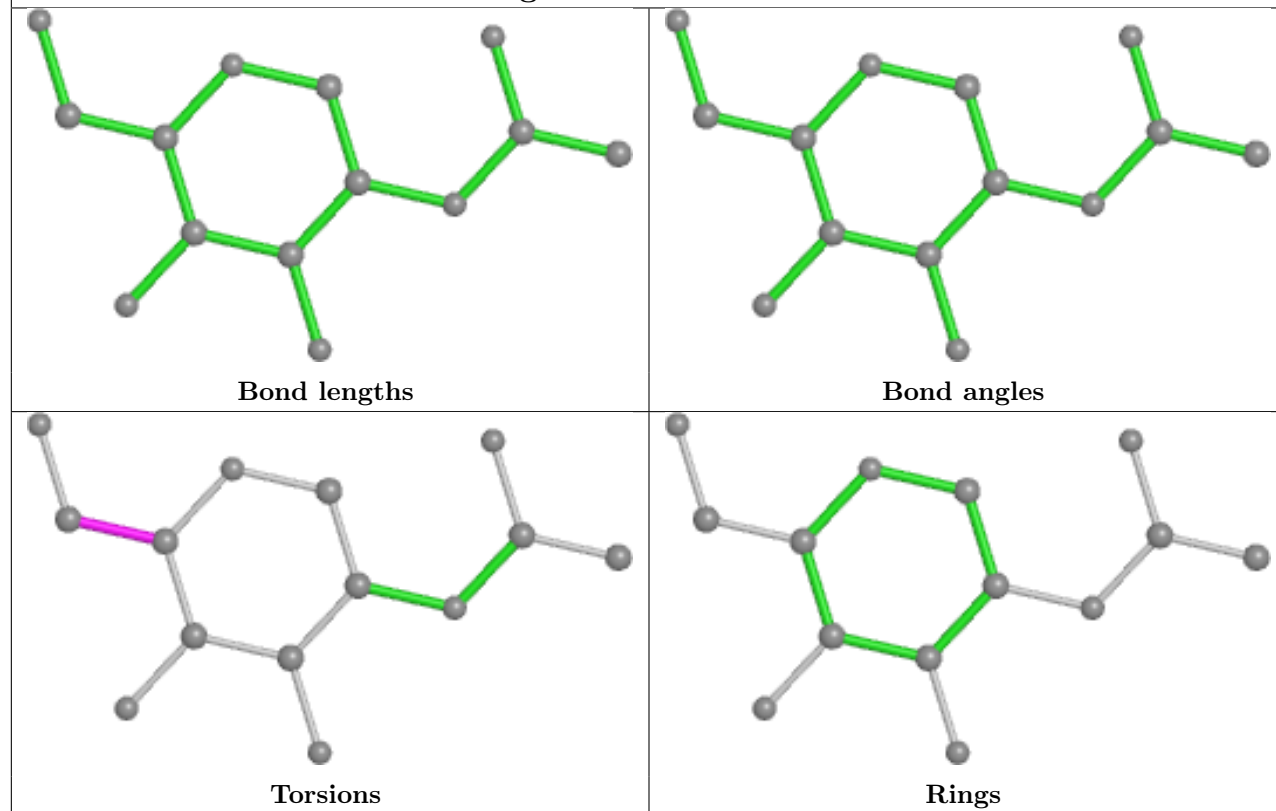
## Ligand NAG C 1212



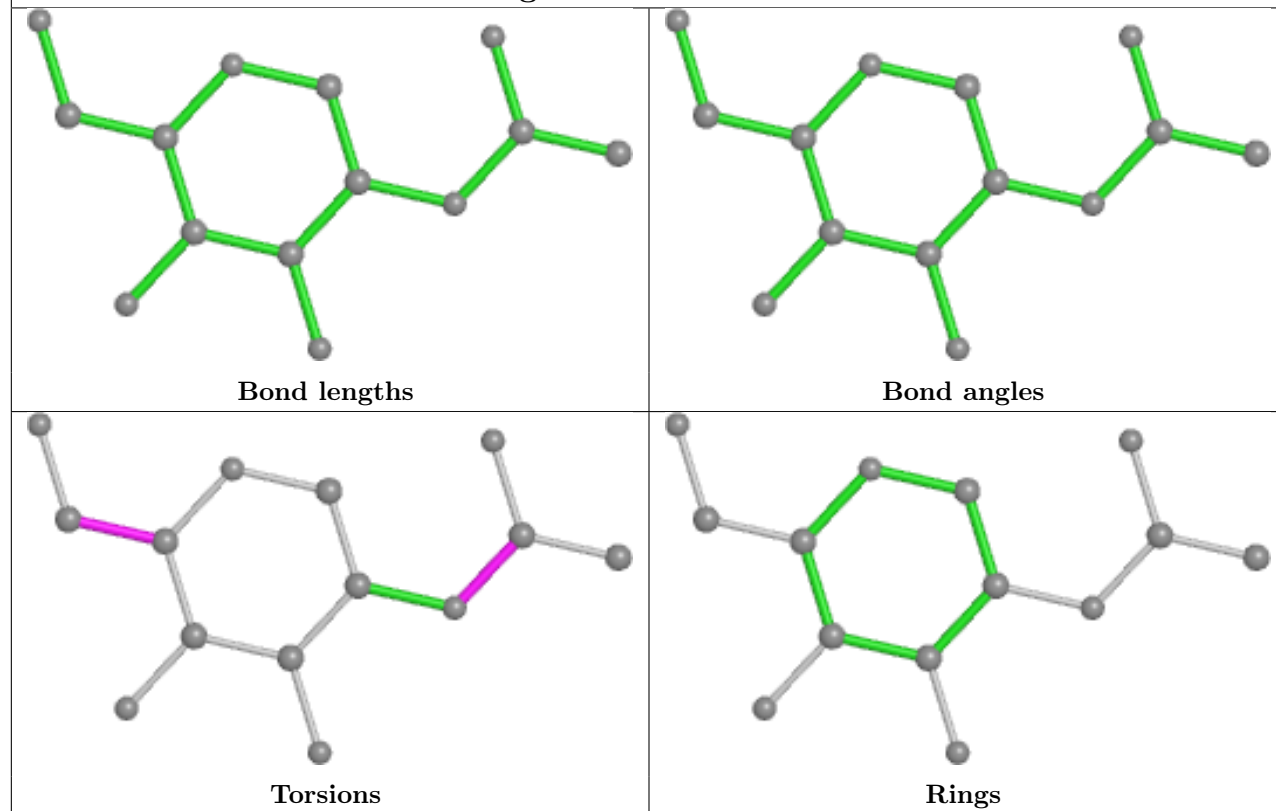




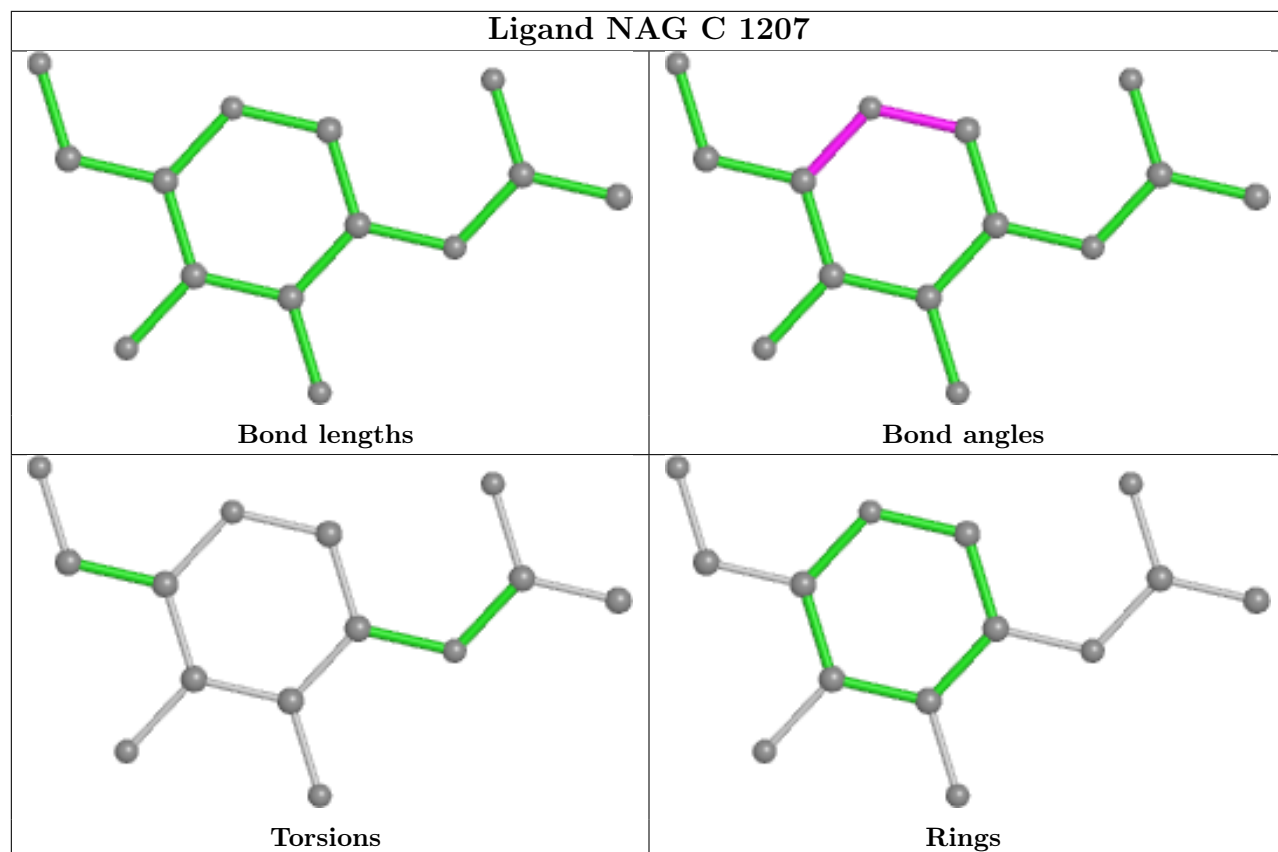
## Ligand NAG B 1212



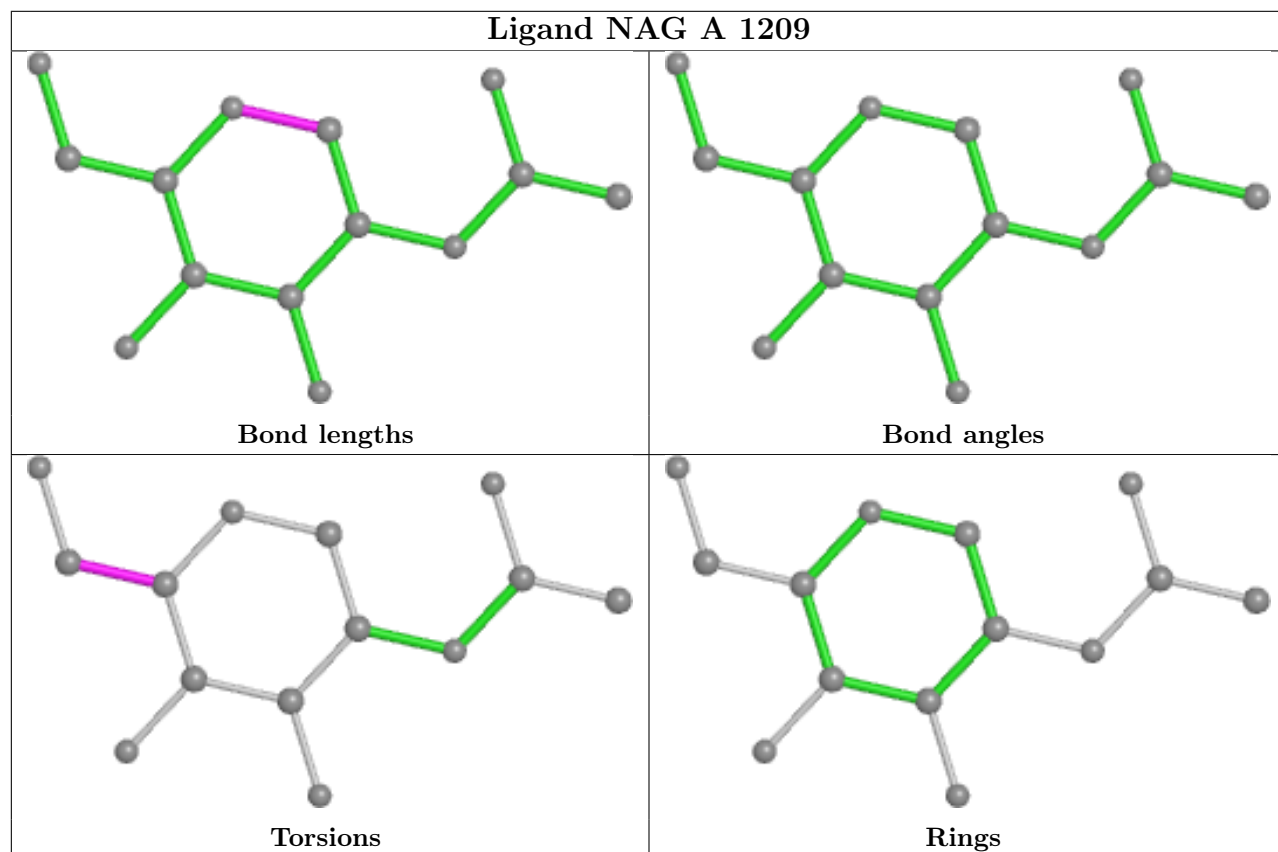
## Ligand NAG C 1215



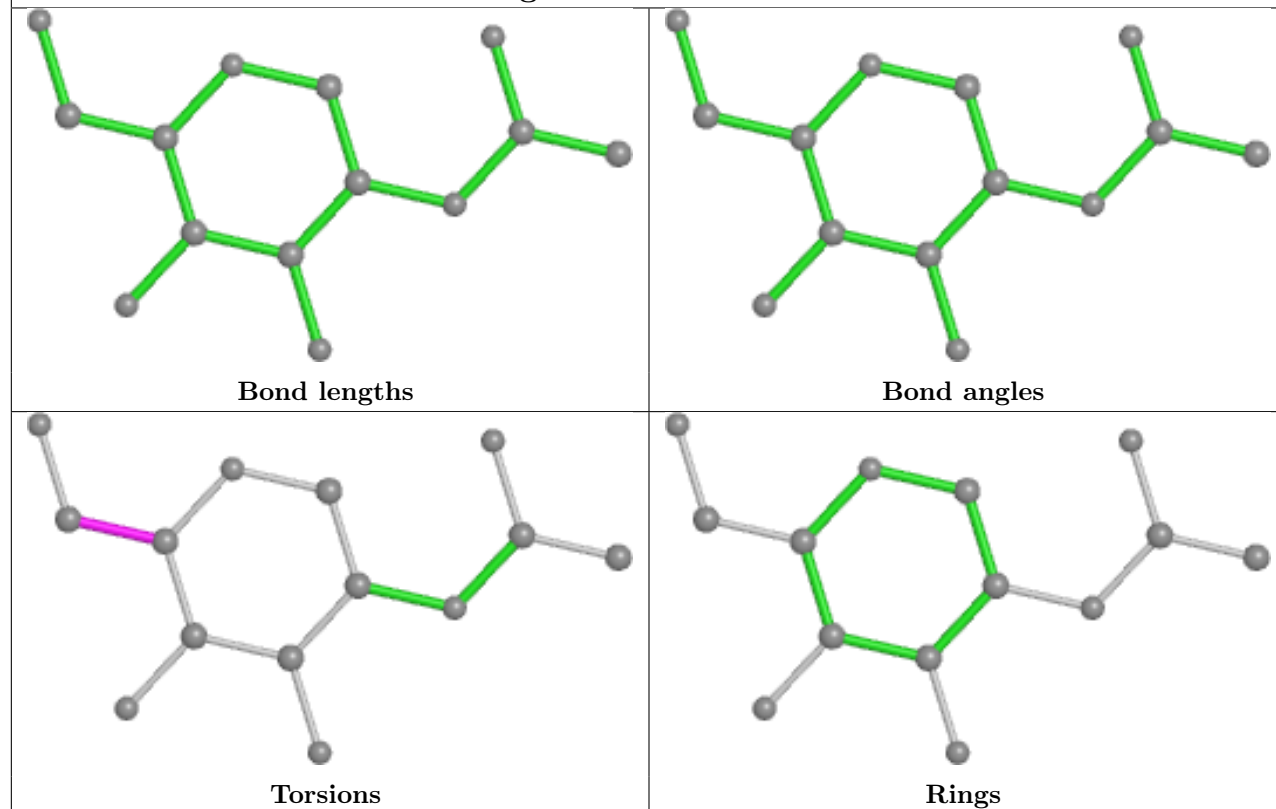
## Ligand NAG C 1207



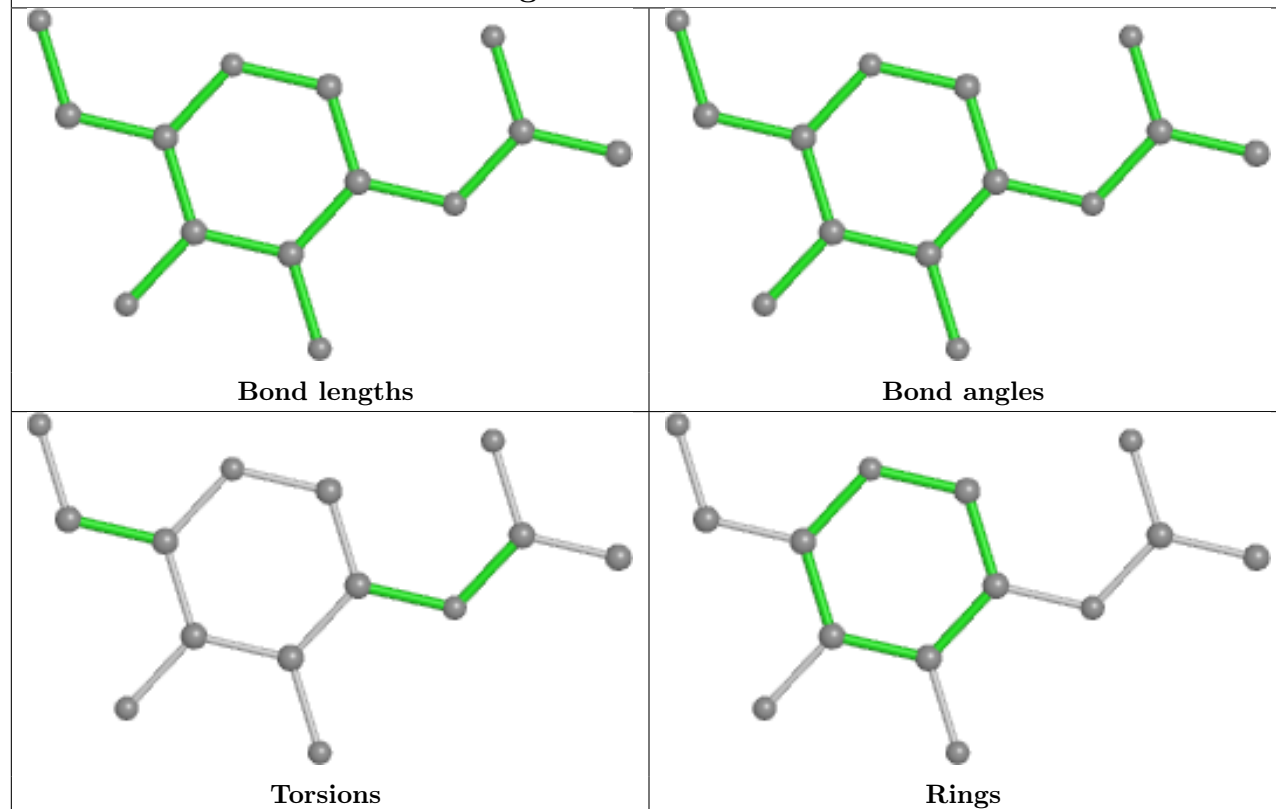
## Ligand NAG A 1209



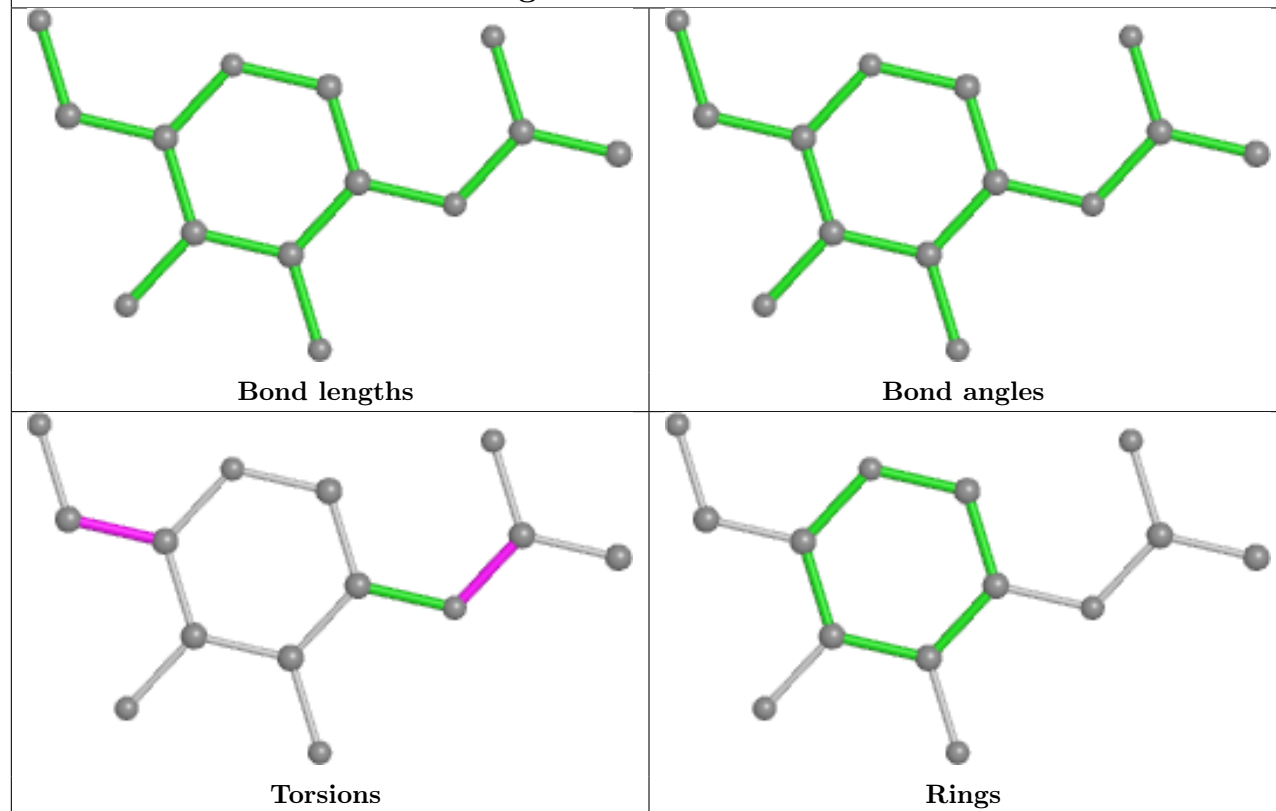
## Ligand NAG B 1206



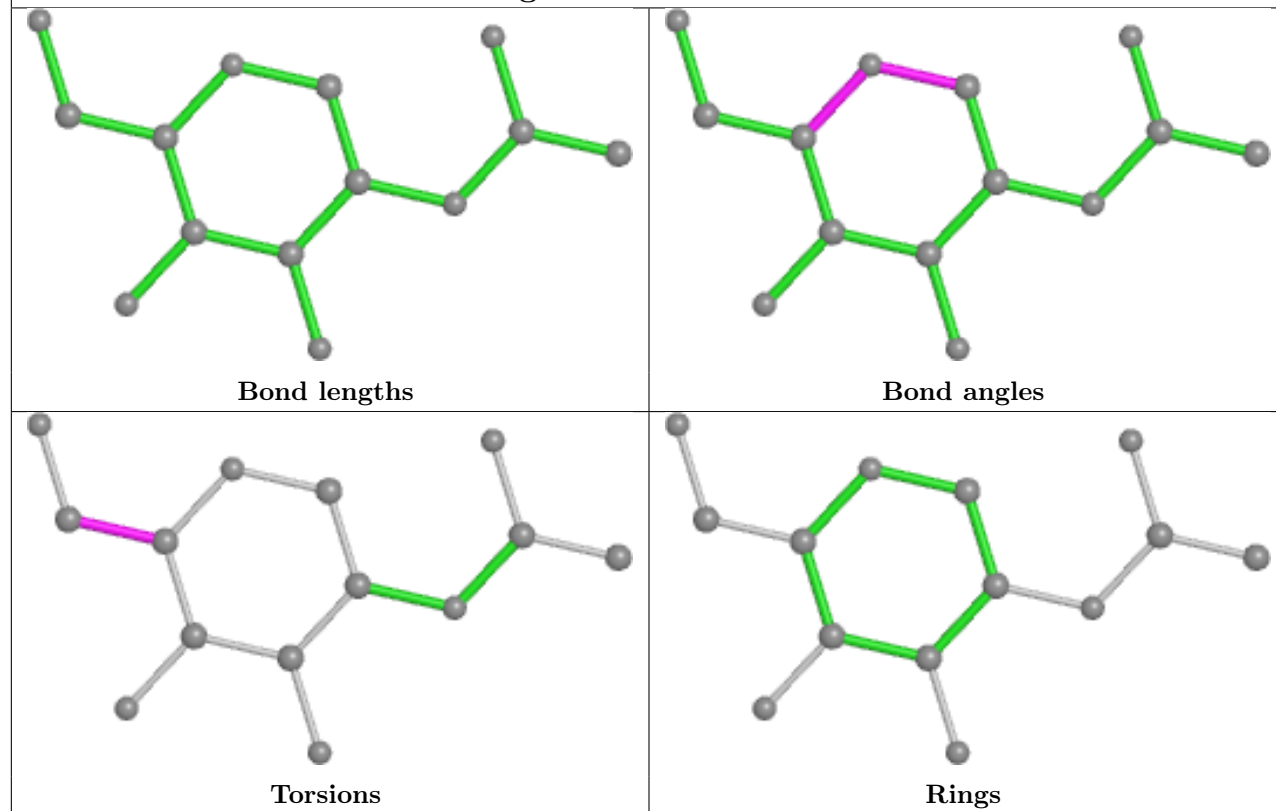
## Ligand NAG C 1204



## Ligand NAG A 1215



## Ligand NAG C 1213



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30496. These allow visual inspection of the internal detail of the map and identification of artifacts.

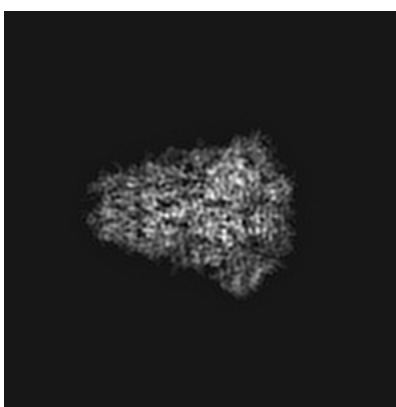
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

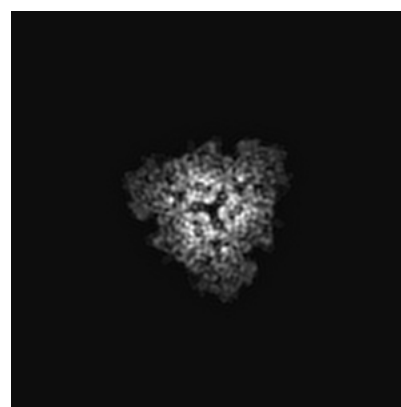
#### 6.1.1 Primary map



X



Y



Z

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

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

#### 6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

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: 89



Y Index: 105

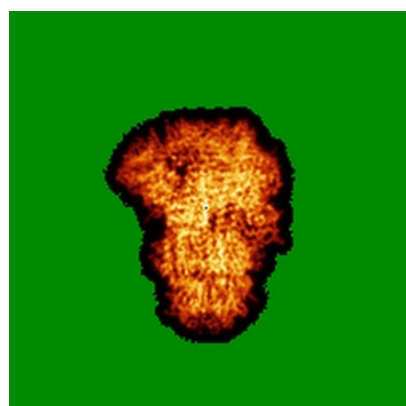


Z Index: 110

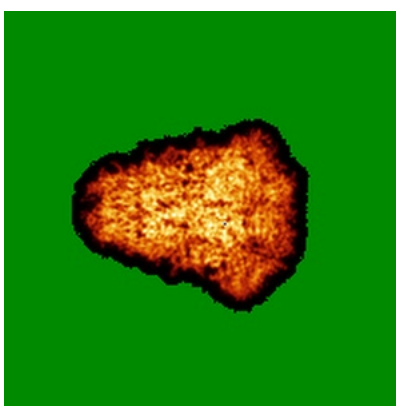
The images above show the largest variance slices of the map in three orthogonal directions.

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

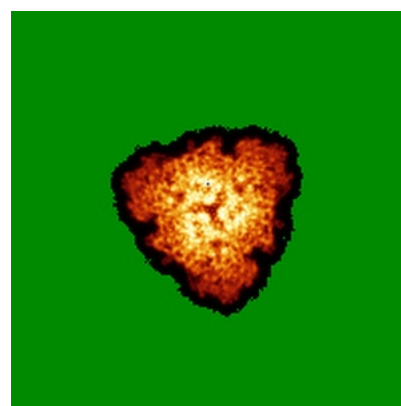
### 6.4.1 Primary map



X



Y



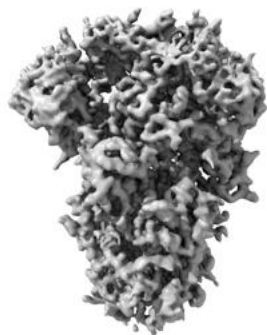
Z

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

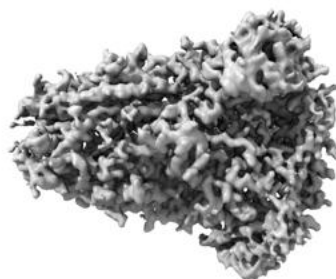


## 6.5 Orthogonal surface views [i](#)

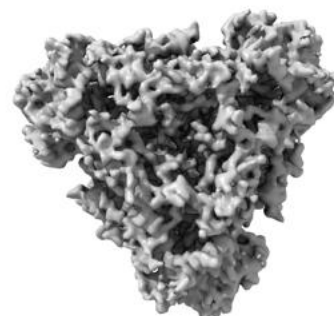
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

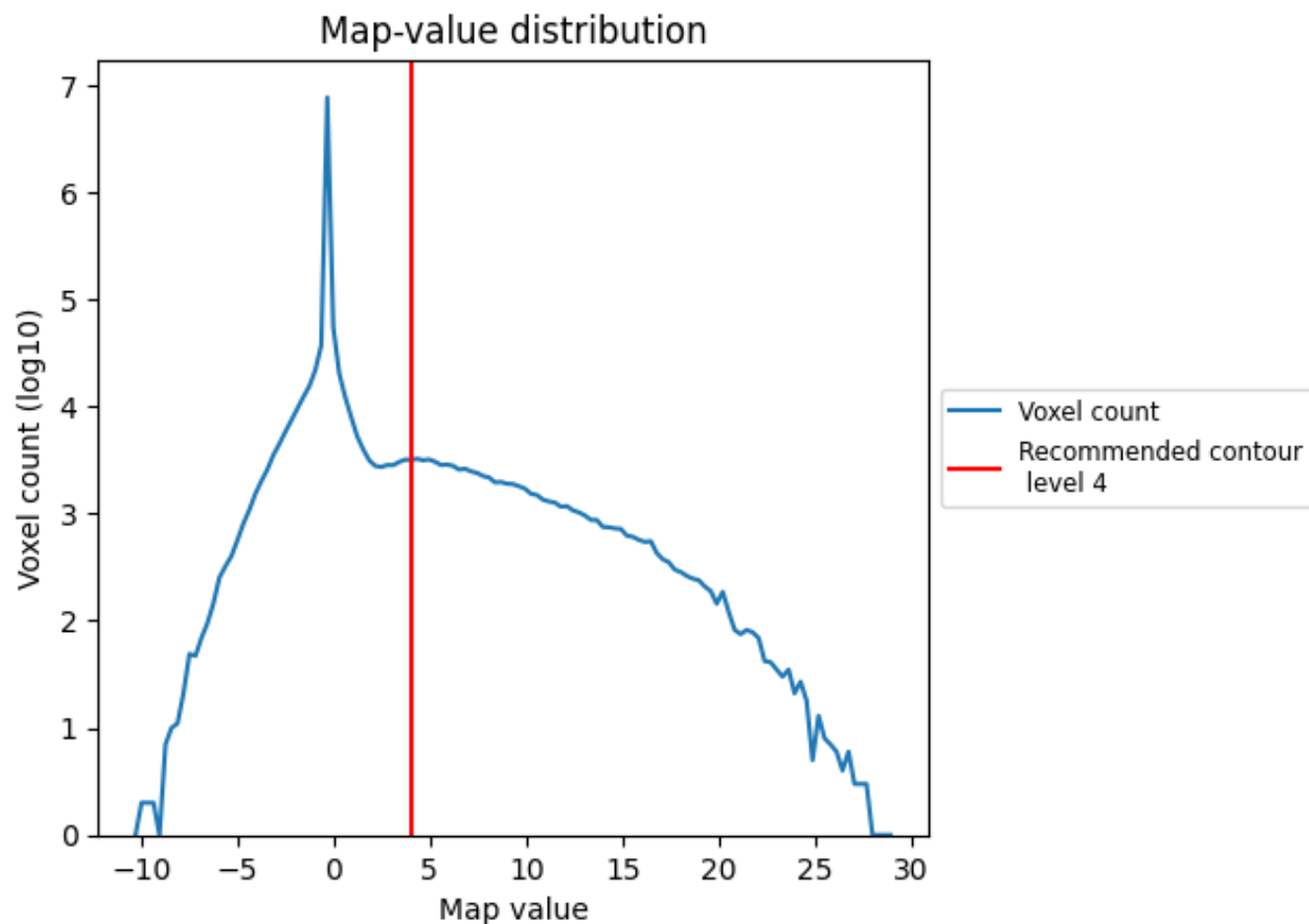
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

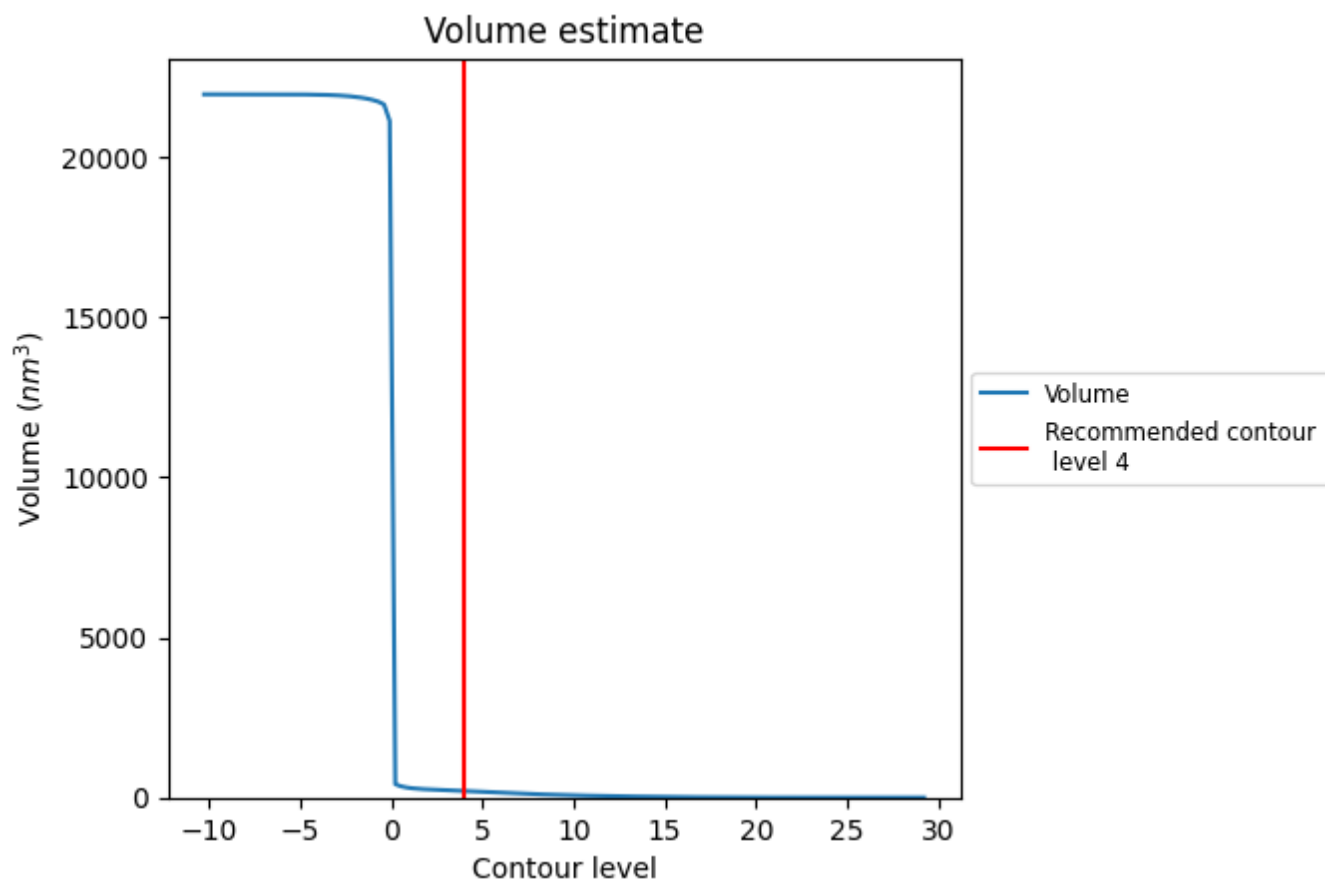
This section contains the results of statistical analysis of the map.

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



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

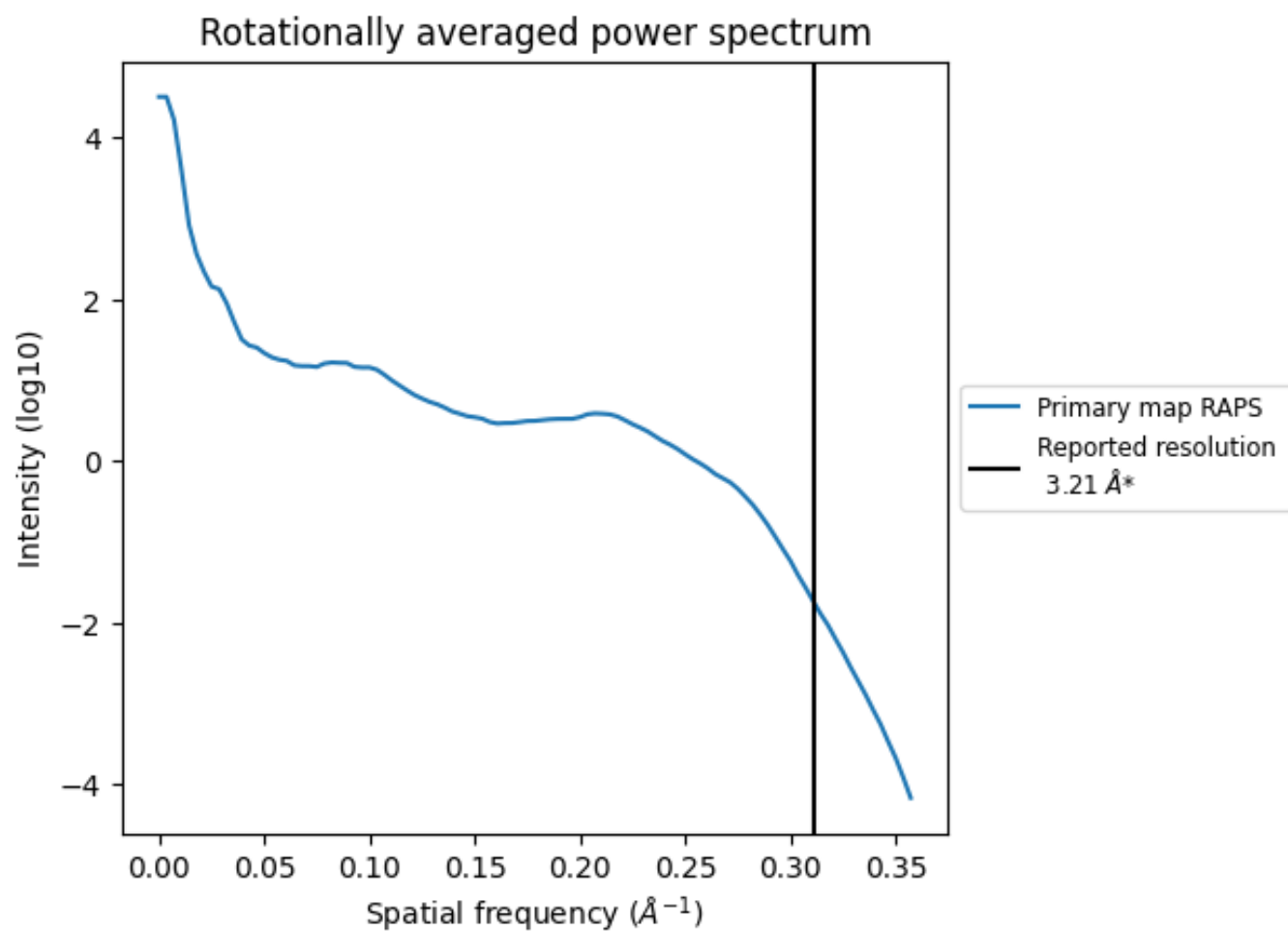
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm<sup>3</sup>; this corresponds to an approximate mass of 184 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

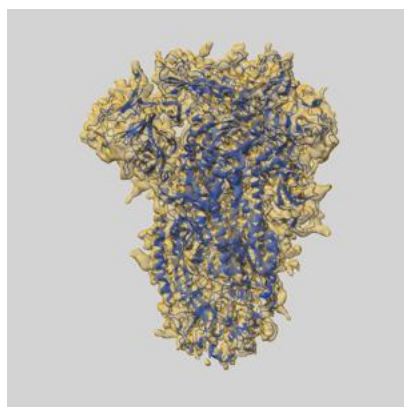
## 8 Fourier-Shell correlation ⓘ

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

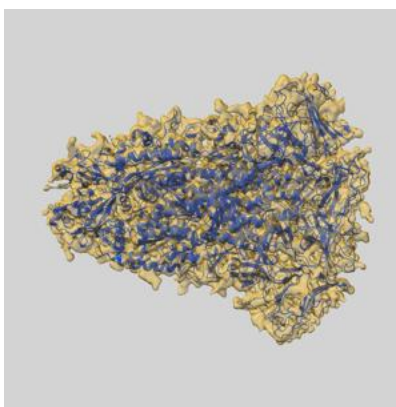
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30496 and PDB model 7CYC. Per-residue inclusion information can be found in section [3](#) on page [9](#).

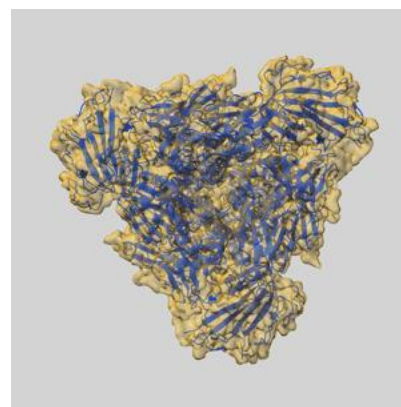
### 9.1 Map-model overlay [i](#)



X



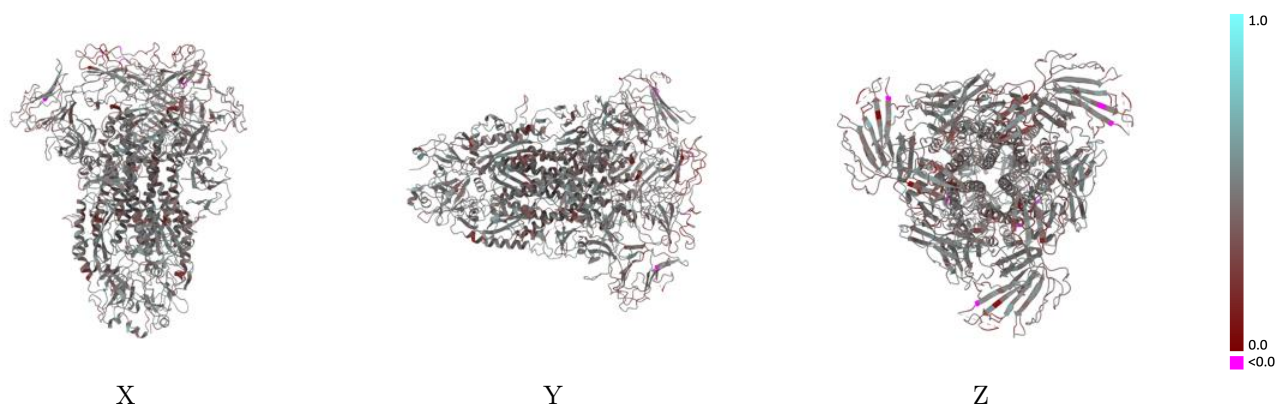
Y



Z

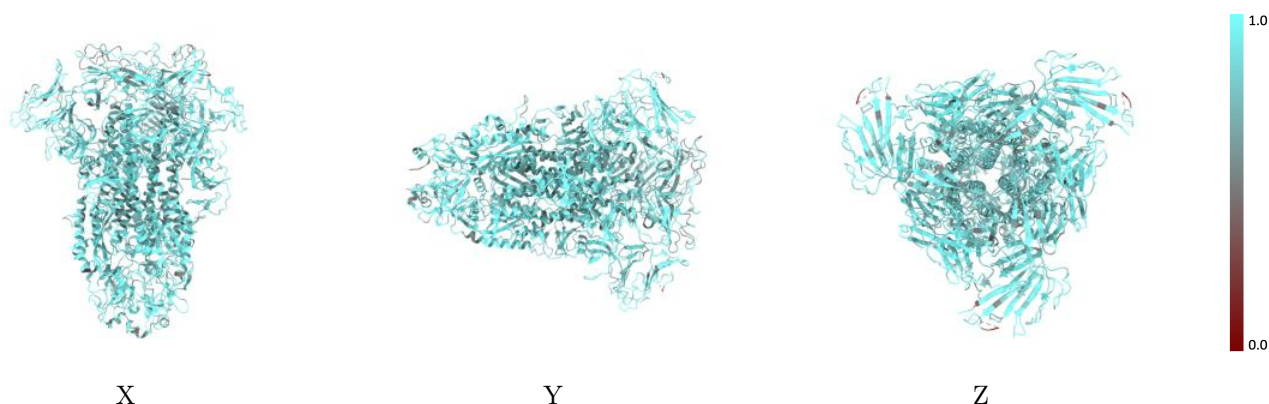
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



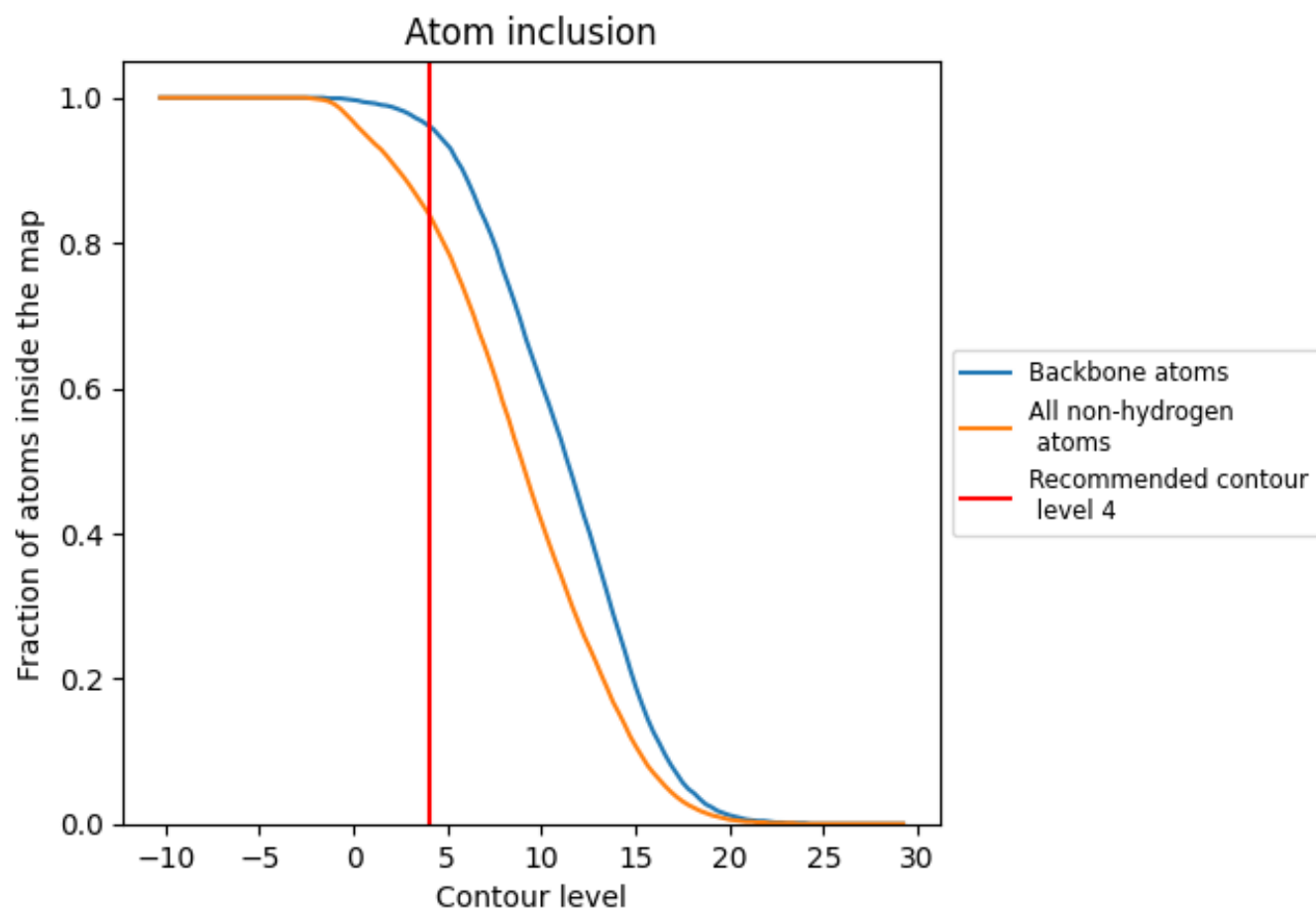
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 84% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8400	<div></div> 0.4240
A	<div></div> 0.8460	<div></div> 0.4280
B	<div></div> 0.8450	<div></div> 0.4270
C	<div></div> 0.8480	<div></div> 0.4260
D	<div></div> 0.5420	<div></div> 0.3230
E	<div></div> 0.6150	<div></div> 0.3120
F	<div></div> 0.4290	<div></div> 0.1820
G	<div></div> 0.7440	<div></div> 0.4220
H	<div></div> 0.5540	<div></div> 0.3310
I	<div></div> 0.5380	<div></div> 0.2800
J	<div></div> 0.3930	<div></div> 0.1950
K	<div></div> 0.7690	<div></div> 0.4430
L	<div></div> 0.5900	<div></div> 0.3190
M	<div></div> 0.5380	<div></div> 0.2550
N	<div></div> 0.3930	<div></div> 0.2380
O	<div></div> 0.7950	<div></div> 0.4320

