



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:47 PM UTC

PDB ID : 7N1Y / pdb_00007n1y
EMDB ID : EMD-24127
Title : Structural basis for enhanced infectivity and immune evasion of SARS-CoV-2 variants
Authors : Zhang, J.; Cai, Y.F.; Xiao, T.S.; Rawson, S.; Peng, H.Q.; Sterling, S.M.; Walsh Jr, R.M.; Volloch, S.R.; Chen, B.
Deposited on : 2021-05-28
Resolution : 4.30 Å (reported)
Based on initial model : 7KRR

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

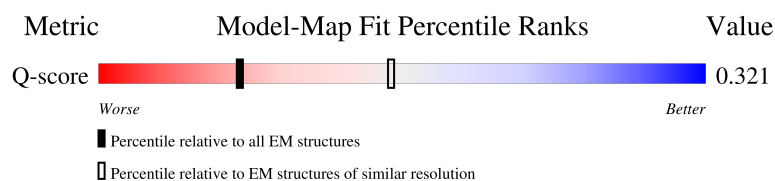
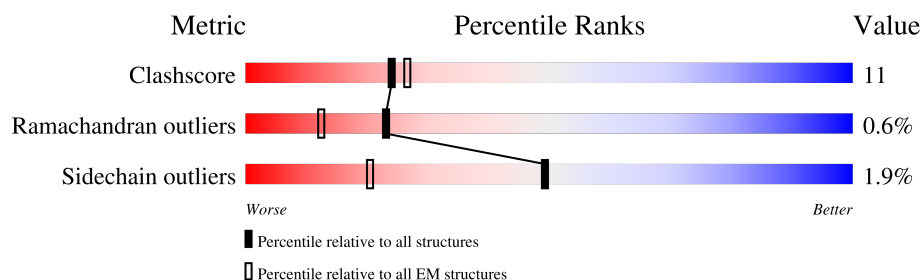
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	A	1305	
1	B	1305	
1	C	1305	

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Mol	Chain	Length	Quality of chain
2	D	2	100%
2	E	2	100%
2	F	2	50% 50%
2	G	2	100%
2	H	2	100%
2	L	2	50% 50%
2	M	2	100%
2	N	2	100%
2	O	2	100%
2	P	2	100%
2	Q	2	100%
2	U	2	50% 50%
2	V	2	100%
2	W	2	100%
2	X	2	100%
2	Y	2	100%
3	I	3	100%
3	R	3	100%
3	Z	3	100%
4	J	3	33% 67%
4	K	3	100%
4	S	3	100%
4	T	3	100%
4	a	3	100%
4	b	3	100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 26636 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	1078	Total	C	N	O	S	0	0
			8441	5391	1407	1605	38		
1	B	1087	Total	C	N	O	S	0	0
			8517	5442	1419	1618	38		
1	C	1077	Total	C	N	O	S	0	0
			8434	5387	1406	1603	38		

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	570	ASP	ALA	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	681	HIS	PRO	conflict	UNP P0DTC2
A	716	ILE	THR	conflict	UNP P0DTC2
A	982	ALA	SER	conflict	UNP P0DTC2
A	1118	HIS	ASP	conflict	UNP P0DTC2
A	1274	SER	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	GLY	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	SER	-	expression tag	UNP P0DTC2
A	1279	ALA	-	expression tag	UNP P0DTC2
A	1280	TRP	-	expression tag	UNP P0DTC2
A	1281	SER	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	PRO	-	expression tag	UNP P0DTC2
A	1284	GLN	-	expression tag	UNP P0DTC2
A	1285	PHE	-	expression tag	UNP P0DTC2
A	1286	GLU	-	expression tag	UNP P0DTC2
A	1287	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1288	GLY	-	expression tag	UNP P0DTC2
A	1289	GLY	-	expression tag	UNP P0DTC2
A	1290	GLY	-	expression tag	UNP P0DTC2
A	1291	SER	-	expression tag	UNP P0DTC2
A	1292	GLY	-	expression tag	UNP P0DTC2
A	1293	GLY	-	expression tag	UNP P0DTC2
A	1294	GLY	-	expression tag	UNP P0DTC2
A	1295	SER	-	expression tag	UNP P0DTC2
A	1296	GLY	-	expression tag	UNP P0DTC2
A	1297	GLY	-	expression tag	UNP P0DTC2
A	1298	SER	-	expression tag	UNP P0DTC2
A	1299	SER	-	expression tag	UNP P0DTC2
A	1300	ALA	-	expression tag	UNP P0DTC2
A	1301	TRP	-	expression tag	UNP P0DTC2
A	1302	SER	-	expression tag	UNP P0DTC2
A	1303	HIS	-	expression tag	UNP P0DTC2
A	1304	PRO	-	expression tag	UNP P0DTC2
A	1305	GLN	-	expression tag	UNP P0DTC2
A	1306	PHE	-	expression tag	UNP P0DTC2
A	1307	GLU	-	expression tag	UNP P0DTC2
A	1308	LYS	-	expression tag	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	570	ASP	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	681	HIS	PRO	conflict	UNP P0DTC2
B	716	ILE	THR	conflict	UNP P0DTC2
B	982	ALA	SER	conflict	UNP P0DTC2
B	1118	HIS	ASP	conflict	UNP P0DTC2
B	1274	SER	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	GLY	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	SER	-	expression tag	UNP P0DTC2
B	1279	ALA	-	expression tag	UNP P0DTC2
B	1280	TRP	-	expression tag	UNP P0DTC2
B	1281	SER	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	PRO	-	expression tag	UNP P0DTC2
B	1284	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1285	PHE	-	expression tag	UNP P0DTC2
B	1286	GLU	-	expression tag	UNP P0DTC2
B	1287	LYS	-	expression tag	UNP P0DTC2
B	1288	GLY	-	expression tag	UNP P0DTC2
B	1289	GLY	-	expression tag	UNP P0DTC2
B	1290	GLY	-	expression tag	UNP P0DTC2
B	1291	SER	-	expression tag	UNP P0DTC2
B	1292	GLY	-	expression tag	UNP P0DTC2
B	1293	GLY	-	expression tag	UNP P0DTC2
B	1294	GLY	-	expression tag	UNP P0DTC2
B	1295	SER	-	expression tag	UNP P0DTC2
B	1296	GLY	-	expression tag	UNP P0DTC2
B	1297	GLY	-	expression tag	UNP P0DTC2
B	1298	SER	-	expression tag	UNP P0DTC2
B	1299	SER	-	expression tag	UNP P0DTC2
B	1300	ALA	-	expression tag	UNP P0DTC2
B	1301	TRP	-	expression tag	UNP P0DTC2
B	1302	SER	-	expression tag	UNP P0DTC2
B	1303	HIS	-	expression tag	UNP P0DTC2
B	1304	PRO	-	expression tag	UNP P0DTC2
B	1305	GLN	-	expression tag	UNP P0DTC2
B	1306	PHE	-	expression tag	UNP P0DTC2
B	1307	GLU	-	expression tag	UNP P0DTC2
B	1308	LYS	-	expression tag	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	570	ASP	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	681	HIS	PRO	conflict	UNP P0DTC2
C	716	ILE	THR	conflict	UNP P0DTC2
C	982	ALA	SER	conflict	UNP P0DTC2
C	1118	HIS	ASP	conflict	UNP P0DTC2
C	1274	SER	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	GLY	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	SER	-	expression tag	UNP P0DTC2
C	1279	ALA	-	expression tag	UNP P0DTC2
C	1280	TRP	-	expression tag	UNP P0DTC2
C	1281	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	PRO	-	expression tag	UNP P0DTC2
C	1284	GLN	-	expression tag	UNP P0DTC2
C	1285	PHE	-	expression tag	UNP P0DTC2
C	1286	GLU	-	expression tag	UNP P0DTC2
C	1287	LYS	-	expression tag	UNP P0DTC2
C	1288	GLY	-	expression tag	UNP P0DTC2
C	1289	GLY	-	expression tag	UNP P0DTC2
C	1290	GLY	-	expression tag	UNP P0DTC2
C	1291	SER	-	expression tag	UNP P0DTC2
C	1292	GLY	-	expression tag	UNP P0DTC2
C	1293	GLY	-	expression tag	UNP P0DTC2
C	1294	GLY	-	expression tag	UNP P0DTC2
C	1295	SER	-	expression tag	UNP P0DTC2
C	1296	GLY	-	expression tag	UNP P0DTC2
C	1297	GLY	-	expression tag	UNP P0DTC2
C	1298	SER	-	expression tag	UNP P0DTC2
C	1299	SER	-	expression tag	UNP P0DTC2
C	1300	ALA	-	expression tag	UNP P0DTC2
C	1301	TRP	-	expression tag	UNP P0DTC2
C	1302	SER	-	expression tag	UNP P0DTC2
C	1303	HIS	-	expression tag	UNP P0DTC2
C	1304	PRO	-	expression tag	UNP P0DTC2
C	1305	GLN	-	expression tag	UNP P0DTC2
C	1306	PHE	-	expression tag	UNP P0DTC2
C	1307	GLU	-	expression tag	UNP P0DTC2
C	1308	LYS	-	expression tag	UNP P0DTC2

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



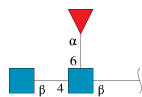
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		

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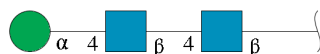
Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		

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



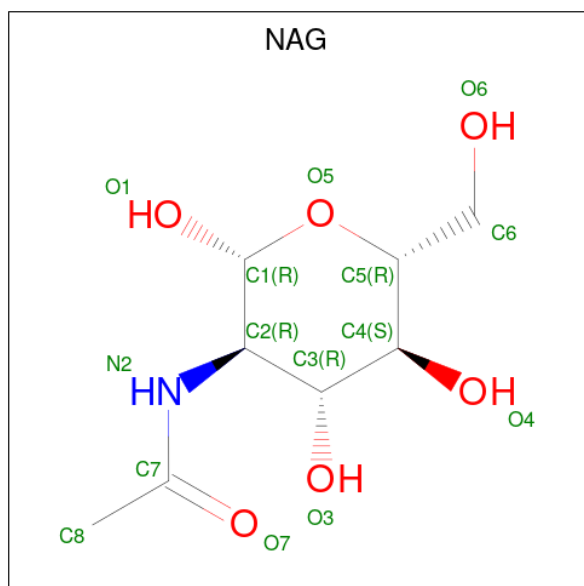
Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	3	Total	C	N	O	0	0
			38	22	2	14		
3	R	3	Total	C	N	O	0	0
			38	22	2	14		
3	Z	3	Total	C	N	O	0	0
			38	22	2	14		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	3	Total	C	N	O	0	0
			39	22	2	15		
4	K	3	Total	C	N	O	0	0
			39	22	2	15		
4	S	3	Total	C	N	O	0	0
			39	22	2	15		
4	T	3	Total	C	N	O	0	0
			39	22	2	15		
4	a	3	Total	C	N	O	0	0
			39	22	2	15		
4	b	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (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	

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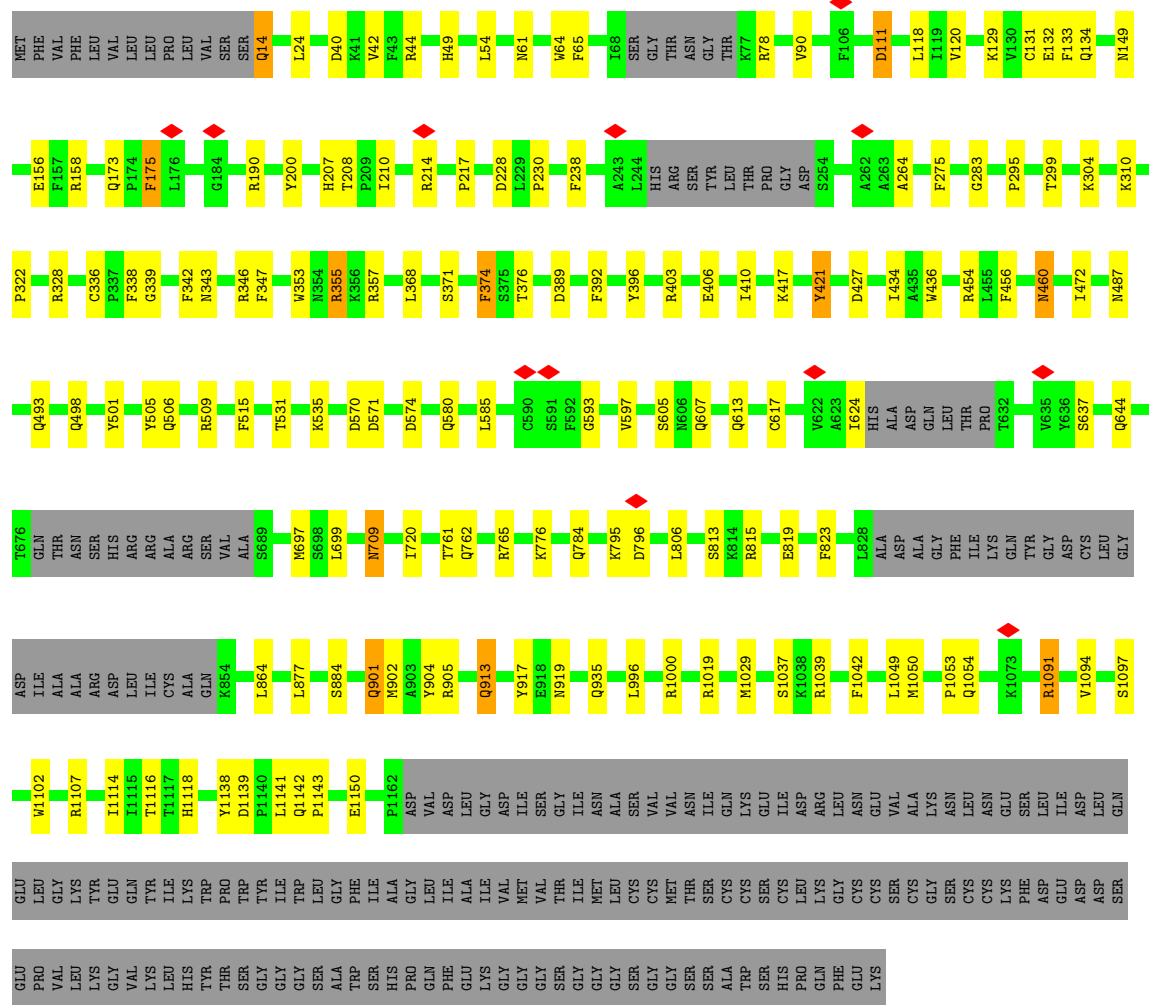
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5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

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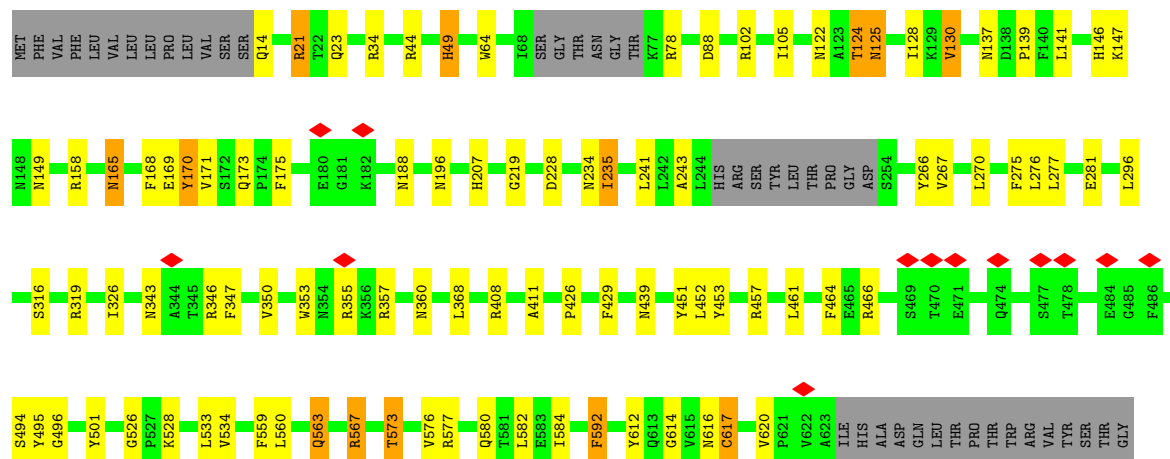
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

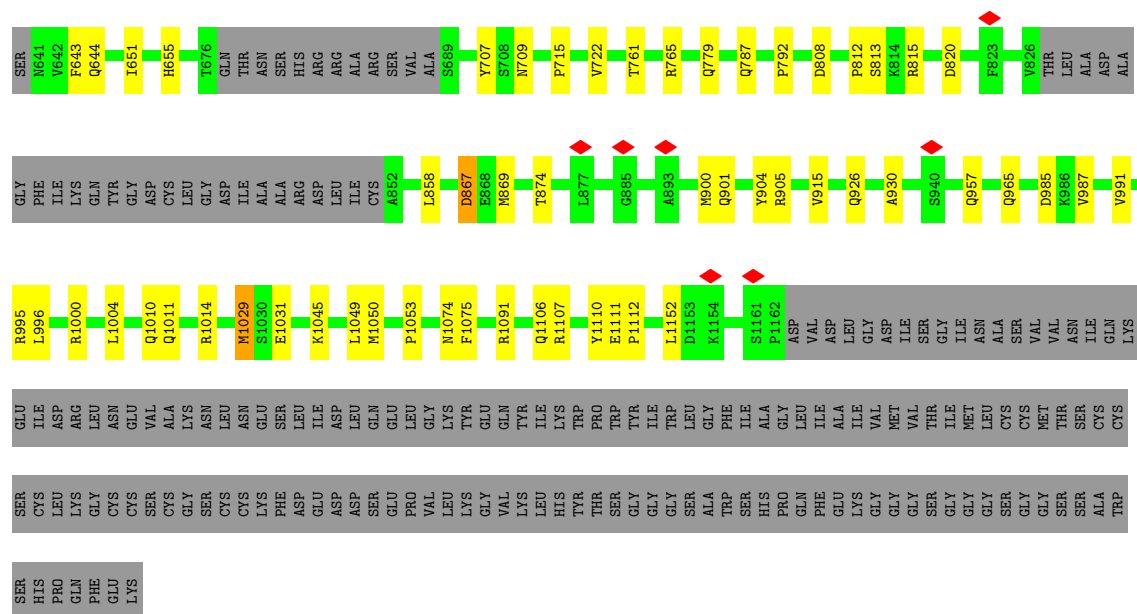
Chain B: 



• Molecule 1: Spike glycoprotein

Chain C: 





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

Chain D: 100%

NAG1
NAG2

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

Chain E: 100%

NAG1
NAG2

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

Chain F: 50% 50%

NAG1
NAG2

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

Chain G: 100%

NAG1
NAG2

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

Chain H:  100%

MAG1
MAG2

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

Chain L:  50% 50%

MAG1
MAG2

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

Chain M:  100%

MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

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

Chain O:  100%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

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

Chain Q:  100%

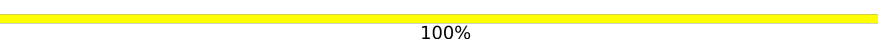
MAG1
MAG2

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

Chain U:  50% 50%

MAG1
MAG2

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

Chain V:  100%

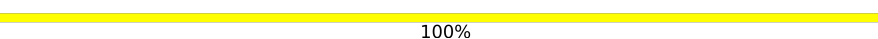
MAG1
MAG2

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

Chain W:  100%

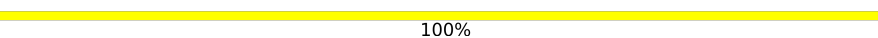
MAG1
MAG2

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

Chain X:  100%

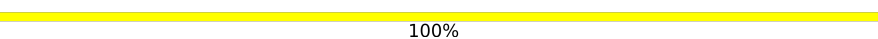
MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2
FUC3

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

Chain R:  100%

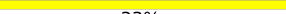
MAG1
MAG2
FUC3

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

Chain Z:  100%

MAG1
MAG2
FUC3

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

Chain J:  33%  67%

MAG1
MAG2
MAN3

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

Chain K:  100%

MAG1
MAG2
MAN3

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

Chain S:  100%

MAG1
MAG2
MAN3

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

Chain T:  100%

MAG1
MAG2
MAN3

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

Chain a:  100%

MAG1
MAG2
MAN3

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

Chain b:

100%

MAG1
MAG2
MAN3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7368	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 ($e^-/\text{\AA}^2$)	53.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.792	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	396.03217, 396.03217, 396.03217	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825067, 0.825067, 0.825067	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.89	0/8636	1.47	51/11746 (0.4%)
1	B	0.89	0/8715	1.46	46/11855 (0.4%)
1	C	0.90	3/8629 (0.0%)	1.45	49/11736 (0.4%)
All	All	0.89	3/25980 (0.0%)	1.46	146/35337 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	985	ASP	CA-C	7.60	1.56	1.52
1	C	792	PRO	CA-C	6.05	1.55	1.51
1	C	995	ARG	CA-C	-5.35	1.46	1.52

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1091	ARG	N-CA-C	-11.81	97.92	111.03
1	B	374	PHE	N-CA-C	9.31	123.84	109.96
1	A	559	PHE	CA-CB-CG	8.90	122.70	113.80
1	A	1091	ARG	N-CA-C	-8.74	101.70	111.14
1	A	149	ASN	OD1-CG-ND2	-8.35	114.25	122.60
1	C	1074	ASN	OD1-CG-ND2	-8.18	114.42	122.60
1	A	40	ASP	CA-CB-CG	7.65	120.25	112.60
1	C	275	PHE	CA-CB-CG	7.60	121.40	113.80
1	A	657	ASN	CB-CG-ND2	7.58	127.78	116.40
1	A	657	ASN	OD1-CG-ND2	-7.47	115.13	122.60
1	A	505	TYR	N-CA-C	-7.29	102.31	112.45
1	A	458	LYS	N-CA-C	-7.20	103.12	110.97
1	A	501	TYR	N-CA-C	7.13	119.94	110.53
1	C	21	ARG	N-CA-C	7.10	117.35	108.19
1	A	149	ASN	CB-CG-ND2	7.02	126.93	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1091	ARG	N-CA-C	-7.01	103.71	112.90
1	A	318	PHE	N-CA-C	6.85	120.62	110.48
1	C	1074	ASN	CB-CG-ND2	6.81	126.62	116.40
1	A	339	GLY	N-CA-C	-6.75	104.67	112.50
1	B	796	ASP	CA-CB-CG	6.51	119.11	112.60
1	C	926	GLN	OE1-CD-NE2	-6.46	116.14	122.60
1	B	574	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	319	ARG	N-CA-C	6.43	117.06	108.38
1	B	493	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	C	592	PHE	CA-CB-CG	6.39	120.19	113.80
1	C	901	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	B	175	PHE	CA-CB-CG	6.26	120.06	113.80
1	C	173	GLN	OE1-CD-NE2	-6.26	116.34	122.60
1	A	979	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	65	PHE	CA-CB-CG	6.19	119.99	113.80
1	B	40	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	655	HIS	CB-CG-CD2	-6.18	123.17	131.20
1	A	23	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	A	917	TYR	N-CA-C	6.15	120.63	113.18
1	C	559	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	969	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	C	567	ARG	N-CA-C	6.09	118.66	109.41
1	B	456	PHE	CA-CB-CG	6.01	119.81	113.80
1	C	787	GLN	OE1-CD-NE2	-6.01	116.58	122.60
1	C	267	VAL	CA-C-N	5.97	126.72	121.58
1	C	267	VAL	C-N-CA	5.97	126.72	121.58
1	A	543	PHE	CA-CB-CG	5.97	119.77	113.80
1	B	784	GLN	OE1-CD-NE2	-5.97	116.63	122.60
1	C	614	GLY	CA-C-N	5.96	129.08	120.98
1	C	614	GLY	C-N-CA	5.96	129.08	120.98
1	A	438	SER	CA-C-N	5.93	129.03	120.38
1	A	438	SER	C-N-CA	5.93	129.03	120.38
1	B	644	GLN	OE1-CD-NE2	-5.89	116.70	122.60
1	A	271	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	B	506	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	C	995	ARG	O-C-N	5.87	128.92	122.11
1	C	360	ASN	CA-CB-CG	5.86	118.46	112.60
1	A	21	ARG	N-CA-C	5.85	119.12	110.46
1	A	861	LEU	CB-CA-C	5.84	117.63	108.88
1	B	593	GLY	CA-C-N	5.82	125.87	120.34
1	B	593	GLY	C-N-CA	5.82	125.87	120.34
1	C	165	ASN	CA-CB-CG	5.79	118.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	563	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	A	309	GLU	CA-C-N	5.75	129.28	121.05
1	A	309	GLU	C-N-CA	5.75	129.28	121.05
1	A	574	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	389	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	460	ASN	CA-CB-CG	5.68	118.28	112.60
1	B	173	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	A	804	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	C	526	GLY	CA-C-N	5.63	125.39	119.76
1	C	526	GLY	C-N-CA	5.63	125.39	119.76
1	B	346	ARG	N-CA-C	5.55	117.45	108.41
1	B	355	ARG	N-CA-C	5.51	117.67	108.02
1	A	925	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	820	ASP	CA-CB-CG	-5.48	107.12	112.60
1	B	217	PRO	N-CA-CB	5.47	107.68	103.30
1	A	1011	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	C	715	PRO	CA-C-N	5.46	129.28	120.82
1	C	715	PRO	C-N-CA	5.46	129.28	120.82
1	B	607	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	B	613	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	954	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	C	170	TYR	N-CA-C	5.42	116.87	107.93
1	C	808	ASP	CA-C-N	5.41	125.23	119.28
1	C	808	ASP	C-N-CA	5.41	125.23	119.28
1	B	322	PRO	CA-C-N	5.41	128.54	120.31
1	B	322	PRO	C-N-CA	5.41	128.54	120.31
1	A	125	ASN	CA-CB-CG	5.41	118.01	112.60
1	B	913	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	C	1074	ASN	CA-CB-CG	5.39	117.99	112.60
1	B	637	SER	CA-C-N	5.39	127.50	120.28
1	B	637	SER	C-N-CA	5.39	127.50	120.28
1	A	493	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	B	570	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	427	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	901	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	B	919	ASN	CA-CB-CG	5.33	117.93	112.60
1	C	357	ARG	N-CA-C	5.32	118.89	109.96
1	C	426	PRO	CA-C-N	5.31	127.93	120.28
1	C	426	PRO	C-N-CA	5.31	127.93	120.28
1	C	965	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	C	1045	LYS	CA-C-N	5.30	128.09	120.56
1	C	1045	LYS	C-N-CA	5.30	128.09	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	PHE	CA-CB-CG	5.29	119.09	113.80
1	C	533	LEU	CA-C-N	5.28	127.58	120.50
1	C	533	LEU	C-N-CA	5.28	127.58	120.50
1	B	111	ASP	CA-C-N	5.25	131.57	121.54
1	B	111	ASP	C-N-CA	5.25	131.57	121.54
1	B	472	ILE	CA-C-N	5.24	128.79	121.24
1	B	472	ILE	C-N-CA	5.24	128.79	121.24
1	C	347	PHE	CA-CB-CG	5.24	119.04	113.80
1	A	146	HIS	CB-CG-CD2	-5.22	124.41	131.20
1	B	1142	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	B	61	ASN	CB-CG-ND2	5.22	124.23	116.40
1	C	49	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	A	211	ASN	CA-CB-CG	5.21	117.81	112.60
1	B	1054	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	188	ASN	CA-CB-CG	5.21	117.81	112.60
1	C	23	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	C	137	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	A	269	TYR	N-CA-C	5.17	117.20	110.53
1	B	214	ARG	N-CA-C	5.15	118.78	112.03
1	C	580	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	C	779	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	B	605	SER	N-CA-C	5.14	117.06	108.99
1	A	620	VAL	CA-C-N	5.13	126.25	119.84
1	A	620	VAL	C-N-CA	5.13	126.25	119.84
1	C	576	VAL	O-C-N	-5.12	117.23	123.02
1	B	14	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	B	806	LEU	CA-C-N	5.12	125.39	119.92
1	B	806	LEU	C-N-CA	5.12	125.39	119.92
1	A	217	PRO	N-CA-CB	5.11	107.87	103.27
1	A	149	ASN	CA-C-N	5.09	129.57	122.08
1	A	149	ASN	C-N-CA	5.09	129.57	122.08
1	A	821	LEU	CA-C-N	5.09	127.37	120.65
1	A	821	LEU	C-N-CA	5.09	127.37	120.65
1	A	138	ASP	CA-C-N	5.08	124.98	119.85
1	A	138	ASP	C-N-CA	5.08	124.98	119.85
1	C	146	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	B	1139	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	957	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	C	281	GLU	CA-C-N	5.05	127.05	120.28
1	C	281	GLU	C-N-CA	5.05	127.05	120.28
1	C	439	ASN	N-CA-C	5.05	116.79	111.28
1	B	762	GLN	OE1-CD-NE2	-5.05	117.55	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	942	ALA	CA-C-N	5.03	127.52	120.28
1	A	942	ALA	C-N-CA	5.03	127.52	120.28
1	C	464	PHE	CA-CB-CG	5.02	118.82	113.80
1	A	965	GLN	OE1-CD-NE2	-5.01	117.59	122.60

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	8441	0	8231	234	0
1	B	8517	0	8303	212	0
1	C	8434	0	8220	157	0
2	D	28	0	25	1	0
2	E	28	0	25	0	0
2	F	28	0	25	5	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	L	28	0	25	1	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	U	28	0	25	1	0
2	V	28	0	25	0	0
2	W	28	0	25	6	0
2	X	28	0	25	0	0
2	Y	28	0	25	0	0
3	I	38	0	34	0	0
3	R	38	0	34	0	0
3	Z	38	0	34	0	0
4	J	39	0	34	6	0
4	K	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	39	0	34	0	0
4	T	39	0	34	0	0
4	a	39	0	34	0	0
4	b	39	0	34	0	0
5	A	154	0	143	26	0
5	B	140	0	130	12	0
5	C	154	0	143	12	0
All	All	26636	0	25876	568	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 11.

All (568) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:THR:HA	1:A:58:PHE:CE2	1.14	1.62
1:A:33:THR:CA	1:A:58:PHE:HE2	1.12	1.61
1:B:709:ASN:HD21	5:B:1409:NAG:C1	1.05	1.61
1:A:234:ASN:HD21	5:A:1405:NAG:C1	1.15	1.57
1:C:165:ASN:HD21	5:C:1404:NAG:C1	1.13	1.55
1:A:165:ASN:HD21	5:A:1404:NAG:C1	1.10	1.54
1:B:815:ARG:NH1	1:B:823:PHE:CG	1.76	1.53
1:A:1098:ASN:HD21	4:J:1:NAG:C1	1.16	1.53
1:A:603:ASN:HD21	5:A:1408:NAG:C1	1.25	1.49
1:C:165:ASN:ND2	5:C:1404:NAG:C1	1.74	1.47
1:B:131:CYS:HB3	1:B:133:PHE:CE2	1.50	1.46
1:A:1079:PRO:CB	1:B:917:TYR:HE2	1.26	1.45
1:A:905:ARG:NH1	1:A:1050:MET:HB3	1.30	1.44
1:A:616:ASN:HD22	2:F:1:NAG:C1	1.31	1.44
1:A:616:ASN:ND2	2:F:1:NAG:C1	1.82	1.43
1:A:1079:PRO:HB2	1:B:917:TYR:CE2	1.53	1.42
1:C:616:ASN:HD21	2:W:1:NAG:C1	1.34	1.40
1:C:125:ASN:HD21	1:C:171:VAL:CG1	1.34	1.40
1:A:904:TYR:CE1	1:C:1107:ARG:HD2	1.56	1.40
1:B:343:ASN:HD21	5:B:1406:NAG:C1	1.34	1.39
1:A:905:ARG:NH2	1:A:1050:MET:HE3	1.10	1.38
1:B:709:ASN:ND2	5:B:1409:NAG:C1	1.83	1.37
1:B:131:CYS:HB3	1:B:133:PHE:CZ	1.57	1.37
1:B:131:CYS:CB	1:B:133:PHE:CE2	2.05	1.37
1:B:1138:TYR:OH	1:B:1143:PRO:CG	1.73	1.35
1:A:1098:ASN:ND2	4:J:1:NAG:C1	1.90	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ASN:ND2	5:A:1408:NAG:C1	1.86	1.34
1:B:131:CYS:CB	1:B:133:PHE:CZ	2.12	1.33
1:A:234:ASN:ND2	5:A:1405:NAG:C1	1.89	1.31
1:A:165:ASN:ND2	5:A:1404:NAG:C1	1.94	1.29
1:A:905:ARG:CZ	1:A:1050:MET:HB3	1.60	1.29
1:A:1094:VAL:HB	1:B:904:TYR:OH	1.33	1.27
1:B:417:LYS:HA	1:B:421:TYR:CE1	1.68	1.27
1:A:1079:PRO:CB	1:B:917:TYR:CE2	2.15	1.26
1:A:273:ARG:NH2	1:A:292:ALA:HB3	1.51	1.26
1:B:815:ARG:NH1	1:B:823:PHE:CB	1.98	1.25
1:B:417:LYS:CB	1:B:421:TYR:OH	1.86	1.23
1:A:905:ARG:NH2	1:A:1050:MET:CE	2.02	1.23
1:C:234:ASN:HD21	5:C:1405:NAG:C1	1.52	1.22
1:B:111:ASP:CA	1:B:134:GLN:HE22	1.54	1.20
1:A:337:PRO:HB2	1:A:340:GLU:OE2	1.36	1.20
1:C:616:ASN:ND2	2:W:1:NAG:C1	2.02	1.20
1:B:498:GLN:CG	1:B:501:TYR:HE2	1.54	1.19
1:C:353:TRP:CH2	1:C:355:ARG:NH2	2.09	1.19
1:A:122:ASN:ND2	5:A:1402:NAG:C1	2.05	1.18
1:C:122:ASN:HD21	5:C:1402:NAG:C1	1.56	1.17
1:A:33:THR:CA	1:A:58:PHE:CE2	1.96	1.17
1:B:815:ARG:HH12	1:B:823:PHE:CB	1.53	1.15
1:A:61:ASN:ND2	5:A:1401:NAG:C1	2.10	1.15
1:B:343:ASN:ND2	5:B:1406:NAG:C1	2.09	1.15
1:B:1107:ARG:CG	1:C:904:TYR:OH	1.90	1.14
1:C:125:ASN:ND2	1:C:171:VAL:HG13	1.59	1.14
1:B:498:GLN:HB2	1:B:501:TYR:CD2	1.80	1.14
1:B:417:LYS:HB3	1:B:421:TYR:OH	1.44	1.14
1:C:617:CYS:SG	1:C:644:GLN:HG3	1.87	1.14
1:C:125:ASN:ND2	1:C:171:VAL:CG1	2.10	1.13
1:A:905:ARG:HH21	1:A:1050:MET:CE	1.59	1.13
1:B:901:GLN:OE1	1:B:905:ARG:NH2	1.82	1.12
1:B:498:GLN:HB2	1:B:501:TYR:CE2	1.85	1.12
1:A:33:THR:HA	1:A:58:PHE:CD2	1.84	1.12
1:A:905:ARG:NH1	1:A:1049:LEU:O	1.83	1.12
1:C:234:ASN:ND2	5:C:1405:NAG:C1	2.13	1.11
1:B:200:TYR:CE2	1:B:230:PRO:HB3	1.86	1.10
1:B:156:GLU:HB3	1:B:158:ARG:HD3	1.23	1.10
1:A:102:ARG:HH11	1:A:179:LEU:HG	1.17	1.09
1:A:904:TYR:HE1	1:C:1107:ARG:CD	1.66	1.08
1:A:1079:PRO:HB3	1:B:917:TYR:HE2	1.17	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:HH22	1:A:292:ALA:HB3	0.95	1.08
1:A:577:ARG:NH2	1:A:582:LEU:HD22	1.68	1.08
1:B:1138:TYR:OH	1:B:1143:PRO:HG3	0.91	1.07
1:B:131:CYS:N	1:B:133:PHE:HE2	1.51	1.07
1:B:1107:ARG:NH1	1:C:904:TYR:CD1	2.10	1.07
1:C:122:ASN:ND2	5:C:1402:NAG:C1	2.17	1.07
1:B:111:ASP:HA	1:B:134:GLN:NE2	1.70	1.05
1:A:33:THR:CB	1:A:58:PHE:CE2	2.38	1.05
1:A:1094:VAL:HB	1:B:904:TYR:HH	0.98	1.05
1:B:1138:TYR:CZ	1:B:1143:PRO:HG3	1.92	1.04
1:C:14:GLN:OE1	1:C:158:ARG:NH2	1.91	1.04
1:A:342:PHE:HE1	1:A:434:ILE:HD12	1.18	1.04
1:B:417:LYS:CG	1:B:421:TYR:OH	2.05	1.04
1:A:61:ASN:HD21	5:A:1401:NAG:C1	1.67	1.03
1:B:131:CYS:HB2	1:B:133:PHE:CZ	1.89	1.03
1:B:156:GLU:HA	1:B:158:ARG:NH1	1.73	1.03
1:C:353:TRP:HH2	1:C:355:ARG:NH2	1.51	1.02
2:W:1:NAG:H62	2:W:2:NAG:H82	1.39	1.01
1:A:905:ARG:NH1	1:A:1050:MET:CB	2.22	1.01
1:A:190:ARG:HH11	1:A:207:HIS:HB2	1.26	1.00
1:B:131:CYS:CA	1:B:133:PHE:CE2	2.44	1.00
1:C:124:THR:O	1:C:175:PHE:CE2	2.14	1.00
1:A:122:ASN:HD21	5:A:1402:NAG:C1	1.69	0.99
1:A:903:ALA:HB2	1:A:917:TYR:CE2	1.98	0.99
1:B:905:ARG:NH1	1:B:1050:MET:HB3	1.78	0.98
1:B:111:ASP:C	1:B:134:GLN:HE22	1.72	0.97
1:B:498:GLN:CG	1:B:501:TYR:CE2	2.46	0.96
1:A:318:PHE:CE2	1:A:615:VAL:HG21	2.01	0.96
1:B:328:ARG:HH21	1:B:580:GLN:HB3	1.29	0.96
1:B:111:ASP:HA	1:B:134:GLN:HE22	1.21	0.95
1:A:577:ARG:NH2	1:A:582:LEU:HD13	1.81	0.95
1:B:1138:TYR:HH	1:B:1143:PRO:HG3	1.15	0.95
1:A:996:LEU:O	1:A:1000:ARG:HG3	1.67	0.95
1:B:815:ARG:NH1	1:B:823:PHE:CD1	2.35	0.95
1:B:1107:ARG:HH11	1:C:904:TYR:HD1	1.12	0.95
1:B:111:ASP:C	1:B:134:GLN:NE2	2.24	0.94
2:W:1:NAG:H62	2:W:2:NAG:C8	1.96	0.94
1:B:498:GLN:CB	1:B:501:TYR:CE2	2.50	0.93
1:B:1107:ARG:NH1	1:C:904:TYR:HD1	1.27	0.93
1:A:337:PRO:CB	1:A:340:GLU:OE2	1.97	0.93
1:A:21:ARG:H	1:A:21:ARG:HD3	1.29	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ASN:HD21	1:C:171:VAL:HG13	0.78	0.93
1:B:111:ASP:CA	1:B:134:GLN:NE2	2.27	0.93
1:C:905:ARG:HH12	1:C:1050:MET:HB3	1.32	0.93
1:A:102:ARG:NH1	1:A:179:LEU:HG	1.82	0.92
1:A:904:TYR:HE1	1:C:1107:ARG:HD2	0.90	0.92
1:B:131:CYS:N	1:B:133:PHE:CE2	2.36	0.92
1:A:1010:GLN:HB3	1:A:1014:ARG:NH1	1.84	0.92
1:C:617:CYS:SG	1:C:644:GLN:CG	2.57	0.92
1:A:32:PHE:O	1:A:58:PHE:HD2	1.53	0.92
1:C:905:ARG:NH1	1:C:1050:MET:HB3	1.84	0.91
1:B:1107:ARG:HG2	1:C:904:TYR:OH	0.99	0.91
1:B:200:TYR:HE2	1:B:230:PRO:HB3	1.35	0.90
1:A:905:ARG:NE	1:A:1050:MET:SD	2.45	0.90
1:A:318:PHE:HE2	1:A:615:VAL:HG21	1.37	0.90
1:A:905:ARG:CZ	1:A:1050:MET:CB	2.50	0.89
1:A:905:ARG:CZ	1:A:1050:MET:HE3	2.02	0.89
1:A:1094:VAL:CB	1:B:904:TYR:OH	2.19	0.89
1:B:156:GLU:HA	1:B:158:ARG:HH11	1.29	0.89
1:A:454:ARG:NH1	1:A:467:ASP:O	2.05	0.88
1:A:904:TYR:CE1	1:C:1107:ARG:CD	2.46	0.88
1:B:374:PHE:CE2	1:B:434:ILE:CG2	2.56	0.88
1:B:815:ARG:HH12	1:B:823:PHE:HB3	1.35	0.88
1:A:1098:ASN:ND2	4:J:1:NAG:C2	2.35	0.88
1:B:1091:ARG:HD2	1:B:1118:HIS:O	1.73	0.88
1:B:417:LYS:HA	1:B:421:TYR:CZ	2.08	0.88
1:B:905:ARG:NE	1:B:1050:MET:HE2	1.89	0.88
1:A:903:ALA:HB2	1:A:917:TYR:HE2	1.32	0.87
1:B:913:GLN:O	1:B:917:TYR:HD1	1.57	0.87
1:A:905:ARG:CZ	1:A:1050:MET:SD	2.63	0.87
1:B:417:LYS:CA	1:B:421:TYR:CE1	2.56	0.87
1:B:815:ARG:NH1	1:B:823:PHE:HB2	1.87	0.87
1:C:1106:GLN:NE2	1:C:1111:GLU:OE1	2.08	0.87
1:C:612:TYR:CE1	1:C:651:ILE:HD13	2.09	0.86
1:A:1010:GLN:HB3	1:A:1014:ARG:HH12	1.37	0.86
1:C:353:TRP:CH2	1:C:355:ARG:CZ	2.58	0.86
1:C:709:ASN:OD1	5:C:1410:NAG:H2	1.74	0.86
1:C:125:ASN:ND2	1:C:171:VAL:HG12	1.88	0.86
1:A:118:LEU:CD1	1:A:160:TYR:CE1	2.58	0.85
1:A:157:PHE:CE2	5:A:1402:NAG:O6	2.28	0.85
1:A:603:ASN:ND2	5:A:1408:NAG:O5	2.01	0.85
1:A:740:MET:HB2	1:C:319:ARG:NH2	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:ARG:HH12	1:A:1050:MET:HB3	1.36	0.85
1:A:33:THR:C	1:A:58:PHE:HE2	1.83	0.85
1:B:417:LYS:CA	1:B:421:TYR:CZ	2.59	0.85
1:B:417:LYS:HG2	1:B:421:TYR:OH	1.75	0.85
1:A:118:LEU:CD1	1:A:160:TYR:HE1	1.89	0.85
1:B:200:TYR:CE2	1:B:230:PRO:CB	2.59	0.85
1:B:498:GLN:CD	1:B:501:TYR:CE2	2.55	0.85
1:B:498:GLN:CB	1:B:501:TYR:HE2	1.88	0.84
1:A:234:ASN:CG	5:A:1405:NAG:C1	2.49	0.84
1:A:342:PHE:CE1	1:A:434:ILE:HD12	2.10	0.84
1:B:24:LEU:O	1:B:78:ARG:NH2	2.10	0.84
1:A:234:ASN:HD21	5:A:1405:NAG:C2	1.91	0.84
1:B:417:LYS:HB3	1:B:421:TYR:CZ	2.11	0.84
1:B:498:GLN:HG3	1:B:501:TYR:HE2	1.41	0.83
1:A:914:ASN:O	1:A:918:GLU:HG2	1.78	0.83
1:C:353:TRP:HH2	1:C:355:ARG:CZ	1.91	0.83
1:A:33:THR:HG22	1:A:58:PHE:CE2	2.14	0.83
1:A:34:ARG:NH1	1:A:217:PRO:HG2	1.93	0.83
1:A:616:ASN:HD21	2:F:1:NAG:C1	1.87	0.83
1:C:14:GLN:OE1	1:C:158:ARG:CZ	2.26	0.83
1:C:915:VAL:HG22	1:C:1111:GLU:OE2	1.79	0.83
1:A:341:VAL:HG21	1:A:358:ILE:HD11	1.58	0.82
1:C:453:TYR:CD1	1:C:495:TYR:CZ	2.63	0.82
1:B:417:LYS:HA	1:B:421:TYR:HE1	1.41	0.81
1:B:149:ASN:ND2	5:B:1402:NAG:C1	2.43	0.81
1:B:498:GLN:CD	1:B:501:TYR:HE2	1.89	0.81
1:B:156:GLU:CB	1:B:158:ARG:HD3	2.08	0.81
1:A:1031:GLU:OE1	1:A:1039:ARG:NH1	2.13	0.80
1:A:118:LEU:HD13	1:A:160:TYR:CE1	2.17	0.80
1:C:124:THR:O	1:C:175:PHE:CD2	2.34	0.80
1:A:521:PRO:CB	1:B:200:TYR:CE1	2.64	0.80
1:B:149:ASN:HD22	5:B:1402:NAG:C1	1.93	0.80
1:B:374:PHE:HE2	1:B:434:ILE:CG2	1.93	0.80
1:C:761:THR:O	1:C:765:ARG:HG3	1.82	0.80
1:A:603:ASN:HD21	5:A:1408:NAG:C2	1.95	0.79
1:B:328:ARG:HH21	1:B:580:GLN:CB	1.94	0.79
1:C:353:TRP:O	1:C:466:ARG:NE	2.15	0.79
1:A:33:THR:CG2	1:A:58:PHE:CE2	2.66	0.79
1:B:131:CYS:HB3	1:B:133:PHE:CD2	2.16	0.79
1:C:577:ARG:HB2	1:C:584:ILE:CD1	2.13	0.79
1:B:417:LYS:CB	1:B:421:TYR:CZ	2.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:MET:HB2	1:C:319:ARG:HH21	1.47	0.78
1:B:498:GLN:HB2	1:B:501:TYR:HD2	1.48	0.77
1:C:353:TRP:CZ3	1:C:355:ARG:NH2	2.51	0.77
1:C:612:TYR:CD1	1:C:651:ILE:CD1	2.68	0.77
1:C:577:ARG:HB2	1:C:584:ILE:HD13	1.67	0.77
1:C:21:ARG:HD2	1:C:78:ARG:NH2	2.00	0.76
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.16	0.76
1:A:577:ARG:NH2	1:A:582:LEU:CD2	2.48	0.76
1:A:577:ARG:HH22	1:A:582:LEU:HD13	1.51	0.76
1:B:134:GLN:HA	1:B:134:GLN:HE21	1.50	0.76
1:B:328:ARG:NH2	1:B:580:GLN:CB	2.50	0.75
1:A:342:PHE:HE1	1:A:434:ILE:CD1	1.98	0.75
1:C:612:TYR:HD1	1:C:651:ILE:CD1	2.01	0.74
1:A:905:ARG:CZ	1:A:1050:MET:CE	2.61	0.74
1:A:122:ASN:HD22	5:A:1402:NAG:C1	1.95	0.74
1:C:815:ARG:HD2	1:C:820:ASP:OD1	1.87	0.74
1:B:200:TYR:CD2	1:B:230:PRO:HA	2.22	0.73
1:B:357:ARG:CZ	1:B:396:TYR:HE2	2.02	0.73
1:B:697:MET:HG3	1:C:869:MET:HE1	1.68	0.73
1:A:916:LEU:CD1	1:A:923:ILE:HD13	2.18	0.73
1:A:421:TYR:O	1:A:454:ARG:HD2	1.89	0.73
1:A:796:ASP:HB3	5:C:1410:NAG:H82	1.70	0.73
1:C:905:ARG:HH12	1:C:1050:MET:CB	2.01	0.73
1:A:273:ARG:NH2	1:A:292:ALA:CB	2.44	0.73
1:C:612:TYR:CD1	1:C:651:ILE:HD13	2.23	0.73
1:A:603:ASN:HD22	5:A:1408:NAG:C1	1.98	0.72
1:C:452:LEU:C	1:C:495:TYR:HE1	1.98	0.72
1:A:21:ARG:HD3	1:A:21:ARG:N	2.04	0.72
1:A:903:ALA:CB	1:A:917:TYR:HE2	2.02	0.72
1:A:340:GLU:CD	1:A:340:GLU:H	1.97	0.72
1:B:815:ARG:NH1	1:B:823:PHE:CD2	2.52	0.72
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.21	0.71
1:C:34:ARG:NH2	1:C:219:GLY:HA3	2.04	0.71
1:A:521:PRO:HB2	1:B:200:TYR:CE1	2.26	0.71
1:C:453:TYR:N	1:C:495:TYR:CE1	2.58	0.71
1:A:1079:PRO:HB2	1:B:917:TYR:CD2	2.23	0.71
1:B:374:PHE:HE2	1:B:434:ILE:HG22	1.56	0.71
1:C:346:ARG:HD2	1:C:346:ARG:O	1.91	0.71
1:A:367:VAL:HG11	5:A:1407:NAG:H62	1.73	0.70
1:C:453:TYR:CD1	1:C:495:TYR:CE2	2.79	0.70
1:B:328:ARG:NH2	1:B:580:GLN:HB3	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:PRO:CB	1:B:200:TYR:HE1	2.03	0.70
1:A:367:VAL:HG22	5:A:1407:NAG:H4	1.74	0.70
1:B:1039:ARG:HD3	1:B:1042:PHE:CD2	2.27	0.70
1:A:658:ASN:HB3	1:A:660:TYR:CE2	2.27	0.70
1:A:340:GLU:OE1	1:A:340:GLU:N	2.24	0.69
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.57	0.69
2:W:1:NAG:H62	2:W:2:NAG:C7	2.21	0.69
1:C:319:ARG:HG2	1:C:592:PHE:HB2	1.74	0.69
1:B:156:GLU:CA	1:B:158:ARG:HH11	2.05	0.69
1:B:339:GLY:CA	5:B:1406:NAG:H82	2.22	0.69
1:A:32:PHE:O	1:A:58:PHE:CD2	2.42	0.69
1:B:913:GLN:O	1:B:917:TYR:CD1	2.45	0.69
1:C:353:TRP:CE3	1:C:466:ARG:NH2	2.59	0.69
1:A:367:VAL:HG21	5:A:1407:NAG:O4	1.93	0.69
1:A:577:ARG:NH2	1:A:582:LEU:CD1	2.55	0.69
1:A:577:ARG:HH22	1:A:582:LEU:HD22	1.55	0.69
1:A:61:ASN:HD22	5:A:1401:NAG:C1	2.04	0.69
1:B:709:ASN:CG	5:B:1409:NAG:C1	2.63	0.69
1:B:905:ARG:CZ	1:B:1050:MET:HE2	2.22	0.68
1:C:353:TRP:HZ3	1:C:355:ARG:HE	1.40	0.68
1:A:1010:GLN:O	1:A:1014:ARG:HG3	1.94	0.68
1:A:983:ARG:O	1:A:983:ARG:HD3	1.93	0.68
1:B:902:MET:SD	1:B:905:ARG:HD2	2.33	0.68
1:A:34:ARG:NH2	1:A:189:LEU:HD21	2.08	0.67
1:A:916:LEU:HD13	1:A:923:ILE:HD13	1.76	0.67
1:B:131:CYS:H	1:B:133:PHE:HE2	1.39	0.67
1:B:190:ARG:HD3	1:B:207:HIS:ND1	2.09	0.67
1:C:452:LEU:C	1:C:495:TYR:CE1	2.72	0.67
1:B:901:GLN:CD	1:B:905:ARG:HH21	1.95	0.67
1:A:33:THR:HB	1:A:58:PHE:CZ	2.30	0.67
1:A:1103:PHE:CE1	1:A:1114:ILE:HD13	2.29	0.67
1:B:134:GLN:NE2	1:B:134:GLN:HA	2.09	0.67
1:B:436:TRP:CZ2	1:B:509:ARG:HD3	2.29	0.67
1:C:612:TYR:HE1	1:C:651:ILE:HD13	1.58	0.67
1:A:87:ASN:OD1	1:A:269:TYR:CE1	2.48	0.67
1:A:905:ARG:NH2	1:A:1050:MET:HB3	2.08	0.67
1:A:33:THR:HB	1:A:58:PHE:CE2	2.30	0.67
1:C:915:VAL:CG2	1:C:1111:GLU:OE2	2.43	0.66
1:B:131:CYS:HB2	1:B:133:PHE:CE2	2.15	0.66
1:B:498:GLN:CB	1:B:501:TYR:CD2	2.71	0.66
1:A:902:MET:SD	1:A:905:ARG:HD2	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:MET:CG	1:A:916:LEU:HD21	2.26	0.66
1:B:357:ARG:CZ	1:B:396:TYR:CE2	2.78	0.66
1:A:190:ARG:NH1	1:A:207:HIS:HB2	2.06	0.65
1:A:905:ARG:HH11	1:A:1049:LEU:C	2.03	0.65
1:A:577:ARG:HH21	1:A:582:LEU:HB3	1.61	0.65
1:A:904:TYR:CD1	1:C:1107:ARG:HD2	2.26	0.65
1:C:457:ARG:NH1	1:C:461:LEU:HD23	2.12	0.64
1:B:371:SER:HB3	1:B:374:PHE:CE1	2.32	0.64
1:A:33:THR:HG22	1:A:58:PHE:CD2	2.32	0.64
1:C:102:ARG:HD2	1:C:243:ALA:HB2	1.80	0.64
1:A:318:PHE:CZ	1:A:615:VAL:HG21	2.32	0.64
1:B:131:CYS:HB3	1:B:133:PHE:CE1	2.26	0.64
1:C:353:TRP:HZ3	1:C:355:ARG:NE	1.95	0.63
1:B:328:ARG:HH22	1:B:580:GLN:HG2	1.63	0.63
1:A:797:PHE:CD2	1:C:707:TYR:CE2	2.86	0.63
1:A:905:ARG:HH21	1:A:1050:MET:HE3	0.81	0.63
1:B:371:SER:HB3	1:B:374:PHE:HE1	1.62	0.63
1:B:131:CYS:O	1:B:133:PHE:CD2	2.51	0.63
1:C:353:TRP:CZ3	1:C:355:ARG:CZ	2.81	0.63
1:A:658:ASN:CB	1:A:660:TYR:CE2	2.82	0.63
1:A:903:ALA:HB2	1:A:917:TYR:CZ	2.32	0.63
1:A:913:GLN:O	1:A:917:TYR:HD2	1.81	0.62
1:A:406:GLU:OE1	1:A:495:TYR:OH	2.16	0.62
1:C:453:TYR:N	1:C:495:TYR:HE1	1.96	0.62
2:U:1:NAG:O4	2:U:2:NAG:O7	2.18	0.62
1:B:421:TYR:HD2	1:B:454:ARG:O	1.81	0.62
1:B:761:THR:O	1:B:765:ARG:HG3	1.98	0.62
1:A:1079:PRO:HB3	1:B:917:TYR:CE2	2.04	0.62
1:A:234:ASN:OD1	5:A:1405:NAG:C1	2.48	0.61
1:C:14:GLN:OE1	1:C:158:ARG:NE	2.33	0.61
1:C:122:ASN:OD1	1:C:125:ASN:O	2.17	0.61
1:C:453:TYR:CD1	1:C:495:TYR:CE1	2.88	0.61
1:C:353:TRP:CZ3	1:C:355:ARG:NE	2.68	0.61
1:A:118:LEU:HD11	1:A:160:TYR:HE1	1.65	0.61
1:C:21:ARG:HD2	1:C:78:ARG:HH21	1.64	0.61
1:A:900:MET:HA	1:A:917:TYR:OH	2.01	0.61
1:A:567:ARG:HD2	1:B:42:VAL:HG11	1.81	0.61
1:B:339:GLY:HA2	5:B:1406:NAG:H82	1.81	0.60
2:W:1:NAG:C6	2:W:2:NAG:H82	2.24	0.60
1:B:353:TRP:CZ3	1:B:355:ARG:HB2	2.37	0.60
1:B:815:ARG:CZ	1:B:823:PHE:HB2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1039:ARG:NH1	1:B:1042:PHE:CZ	2.69	0.60
1:A:309:GLU:OE1	1:A:313:TYR:OH	2.16	0.60
1:B:776:LYS:NZ	1:B:1019:ARG:HH22	1.98	0.60
1:A:737:ASP:OD2	1:C:319:ARG:HD3	2.02	0.60
1:B:1138:TYR:OH	1:B:1143:PRO:HG2	1.92	0.60
1:A:521:PRO:HB3	1:B:200:TYR:HE1	1.65	0.59
1:A:797:PHE:HD2	1:C:707:TYR:CZ	2.20	0.59
1:C:102:ARG:NE	1:C:141:LEU:CD2	2.65	0.59
1:A:33:THR:CB	1:A:58:PHE:CZ	2.84	0.59
1:A:916:LEU:HD12	1:A:923:ILE:CD1	2.31	0.59
1:B:131:CYS:HB2	1:B:133:PHE:HZ	1.60	0.59
1:B:374:PHE:CE2	1:B:434:ILE:HG22	2.32	0.59
1:C:496:GLY:O	1:C:501:TYR:HE2	1.85	0.59
1:B:1039:ARG:NH1	1:B:1042:PHE:CE1	2.70	0.59
1:A:1103:PHE:HD1	1:A:1113:GLN:C	2.10	0.59
1:A:1010:GLN:CB	1:A:1014:ARG:HH12	2.13	0.58
1:C:147:LYS:HB3	5:C:1403:NAG:O7	2.03	0.58
1:A:86:PHE:CD1	1:A:235:ILE:HG21	2.38	0.58
1:A:102:ARG:NH1	1:A:178:ASP:O	2.36	0.58
1:A:466:ARG:O	1:A:466:ARG:HG2	2.04	0.58
1:A:1098:ASN:ND2	4:J:1:NAG:H2	2.19	0.57
1:B:498:GLN:HG3	1:B:501:TYR:CE2	2.26	0.57
1:A:905:ARG:NH1	1:A:1049:LEU:C	2.61	0.57
1:C:353:TRP:CZ3	1:C:466:ARG:NH2	2.72	0.57
1:C:1011:GLN:HA	1:C:1014:ARG:HH11	1.68	0.57
1:C:612:TYR:CE1	1:C:620:VAL:HG11	2.39	0.57
1:C:577:ARG:HG3	1:C:582:LEU:O	2.04	0.57
1:C:102:ARG:NE	1:C:141:LEU:HD23	2.19	0.57
1:C:105:ILE:HG12	1:C:241:LEU:HD11	1.85	0.57
1:A:906:PHE:CD1	1:A:916:LEU:HD22	2.40	0.57
1:A:902:MET:HG3	1:A:916:LEU:CD2	2.35	0.57
1:B:1094:VAL:HB	1:C:904:TYR:OH	2.04	0.57
1:B:421:TYR:CD2	1:B:454:ARG:O	2.57	0.57
1:B:374:PHE:CE2	1:B:434:ILE:HG23	2.39	0.56
1:A:86:PHE:CD1	1:A:235:ILE:CG2	2.89	0.56
1:A:318:PHE:HE2	1:A:615:VAL:CG2	2.13	0.56
1:B:343:ASN:CG	5:B:1406:NAG:C1	2.78	0.56
1:C:319:ARG:HG2	1:C:592:PHE:CB	2.35	0.56
1:C:1075:PHE:CE2	1:C:1110:TYR:HE1	2.23	0.56
1:C:643:PHE:CE1	1:C:655:HIS:ND1	2.74	0.56
1:C:408:ARG:NH1	1:C:411:ALA:CB	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:ARG:HH21	1:A:582:LEU:CB	2.19	0.55
1:A:797:PHE:CE2	1:C:707:TYR:CE2	2.94	0.55
1:C:815:ARG:NH2	1:C:867:ASP:OD2	2.39	0.55
1:C:346:ARG:HD2	1:C:346:ARG:C	2.32	0.55
1:B:913:GLN:HB2	1:B:917:TYR:HE1	1.72	0.55
2:D:1:NAG:H5	2:D:2:NAG:C7	2.37	0.55
1:B:498:GLN:OE1	1:B:501:TYR:CE2	2.59	0.55
1:A:21:ARG:H	1:A:21:ARG:CD	2.12	0.55
1:A:740:MET:CB	1:C:319:ARG:HH21	2.19	0.55
1:C:453:TYR:HD1	1:C:495:TYR:CE1	2.25	0.55
1:B:131:CYS:C	1:B:133:PHE:CD2	2.85	0.54
1:B:417:LYS:CA	1:B:421:TYR:OH	2.49	0.54
1:C:1011:GLN:HA	1:C:1014:ARG:NH1	2.22	0.54
1:C:1075:PHE:CE2	1:C:1110:TYR:CE1	2.95	0.54
1:A:101:ILE:HD13	1:A:242:LEU:HG	1.90	0.54
1:A:797:PHE:CD2	1:C:707:TYR:CZ	2.95	0.54
1:B:1039:ARG:NH2	1:C:1031:GLU:OE1	2.39	0.54
1:C:124:THR:O	1:C:175:PHE:CZ	2.59	0.54
1:A:753:LEU:HA	1:A:756:TYR:HD2	1.73	0.54
1:A:903:ALA:HB2	1:A:917:TYR:OH	2.07	0.54
1:A:157:PHE:CZ	5:A:1402:NAG:O6	2.55	0.54
1:A:577:ARG:HH22	1:A:582:LEU:CD1	2.15	0.54
1:A:577:ARG:HH21	1:A:582:LEU:HD22	1.65	0.54
1:B:347:PHE:HE1	1:B:509:ARG:HH21	1.56	0.54
1:A:905:ARG:NH2	1:A:1050:MET:CB	2.69	0.54
1:B:111:ASP:CB	1:B:134:GLN:HE22	2.19	0.54
1:A:501:TYR:HB3	1:A:505:TYR:HB3	1.89	0.54
1:C:996:LEU:O	1:C:1000:ARG:HG3	2.08	0.54
1:A:1103:PHE:CE1	1:A:1114:ILE:CD1	2.91	0.53
1:C:408:ARG:HH12	1:C:411:ALA:CB	2.22	0.53
1:A:740:MET:CB	1:C:319:ARG:NH2	2.66	0.53
1:A:797:PHE:HD2	1:C:707:TYR:OH	1.91	0.53
1:B:328:ARG:NH2	1:B:580:GLN:HG2	2.23	0.53
1:A:337:PRO:HB2	1:A:340:GLU:CD	2.27	0.52
1:A:367:VAL:CG1	5:A:1407:NAG:H62	2.37	0.52
1:C:196:ASN:HD22	1:C:235:ILE:HG22	1.74	0.52
1:B:131:CYS:O	1:B:133:PHE:HD2	1.92	0.52
1:B:342:PHE:CE2	1:B:374:PHE:HZ	2.27	0.52
1:C:612:TYR:HD1	1:C:651:ILE:HD12	1.74	0.52
1:A:902:MET:HG2	1:A:916:LEU:HD21	1.91	0.52
1:A:1098:ASN:CG	4:J:1:NAG:C1	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:TYR:CE2	1:B:230:PRO:CA	2.94	0.52
1:A:646:ARG:HB2	1:A:668:ALA:HB1	1.93	0.51
1:B:328:ARG:NH1	1:B:531:THR:O	2.43	0.51
1:C:813:SER:OG	1:C:815:ARG:NE	2.44	0.51
1:A:644:GLN:NE2	2:F:1:NAG:H82	2.25	0.51
1:A:753:LEU:HA	1:A:756:TYR:CD2	2.45	0.51
1:B:14:GLN:O	1:B:158:ARG:HG3	2.10	0.51
1:B:200:TYR:HD2	1:B:228:ASP:OD1	1.93	0.51
1:A:22:THR:O	1:A:78:ARG:NH1	2.44	0.51
1:A:577:ARG:NH2	1:A:582:LEU:CG	2.73	0.51
1:A:916:LEU:HD12	1:A:923:ILE:HD13	1.91	0.51
1:B:200:TYR:CD2	1:B:228:ASP:OD1	2.64	0.51
1:A:21:ARG:N	1:A:21:ARG:CD	2.73	0.51
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.76	0.51
1:A:577:ARG:HD2	1:A:582:LEU:HB3	1.93	0.50
1:B:815:ARG:HG2	1:B:819:GLU:HB2	1.92	0.50
1:A:421:TYR:HA	1:A:457:ARG:HG3	1.94	0.50
1:C:125:ASN:HA	1:C:175:PHE:CZ	2.46	0.50
1:C:453:TYR:CA	1:C:495:TYR:HE1	2.24	0.50
1:A:577:ARG:HB2	1:A:584:ILE:CD1	2.41	0.50
1:A:367:VAL:CG2	5:A:1407:NAG:H4	2.40	0.50
1:B:129:LYS:HE3	1:B:133:PHE:CZ	2.46	0.50
1:B:299:THR:HG22	1:B:597:VAL:HG11	1.94	0.50
1:B:417:LYS:O	1:B:421:TYR:CE1	2.65	0.50
1:A:355:ARG:HB2	1:A:466:ARG:NH2	2.27	0.49
1:B:392:PHE:CE1	1:B:515:PHE:CD2	3.00	0.49
1:B:421:TYR:CD1	1:B:421:TYR:N	2.80	0.49
1:C:567:ARG:NH1	1:C:573:THR:H	2.10	0.49
1:A:342:PHE:CE1	1:A:434:ILE:CD1	2.83	0.49
1:A:905:ARG:HH12	1:A:1050:MET:CB	2.08	0.49
1:A:916:LEU:HD12	1:A:923:ILE:HD12	1.94	0.49
1:B:776:LYS:HZ2	1:B:1019:ARG:HH22	1.60	0.49
1:C:1106:GLN:NE2	1:C:1111:GLU:CD	2.70	0.49
1:A:118:LEU:HD13	1:A:160:TYR:HE1	1.60	0.49
1:B:1141:LEU:HD23	1:B:1141:LEU:C	2.37	0.49
1:A:567:ARG:CD	1:B:42:VAL:HG11	2.42	0.49
1:B:813:SER:C	1:B:815:ARG:H	2.21	0.49
1:B:1039:ARG:CZ	1:B:1042:PHE:CD1	2.95	0.49
1:C:451:TYR:O	1:C:495:TYR:N	2.41	0.48
1:C:709:ASN:OD1	5:C:1410:NAG:C2	2.43	0.48
1:C:567:ARG:HG2	1:C:573:THR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:GLY:HA3	5:B:1406:NAG:H82	1.95	0.48
1:B:996:LEU:O	1:B:1000:ARG:HG3	2.13	0.48
1:B:905:ARG:NH1	1:B:1050:MET:CB	2.65	0.48
1:B:905:ARG:HH11	1:B:1050:MET:HB3	1.75	0.48
1:B:328:ARG:NH2	1:B:580:GLN:CG	2.76	0.48
1:B:1091:ARG:CD	1:B:1118:HIS:O	2.53	0.48
1:C:1029:MET:HE1	1:C:1053:PRO:HB3	1.96	0.48
1:B:190:ARG:HD2	1:B:207:HIS:HA	1.96	0.48
1:B:905:ARG:CD	1:B:1049:LEU:HG	2.44	0.47
1:B:336:CYS:HB2	1:B:338:PHE:CZ	2.49	0.47
1:C:128:ILE:HG12	1:C:170:TYR:HB3	1.96	0.47
1:A:521:PRO:HB3	1:B:200:TYR:CE1	2.43	0.47
1:A:577:ARG:HH21	1:A:582:LEU:CG	2.28	0.47
1:A:646:ARG:HB2	1:A:668:ALA:CB	2.45	0.47
1:B:815:ARG:CZ	1:B:823:PHE:CB	2.85	0.47
1:A:457:ARG:NH1	1:A:461:LEU:HB3	2.28	0.47
1:B:357:ARG:CD	1:B:396:TYR:CD2	2.98	0.46
1:B:357:ARG:NE	1:B:396:TYR:CE2	2.82	0.46
1:A:1103:PHE:HD1	1:A:1113:GLN:O	1.99	0.46
2:L:1:NAG:H62	2:L:2:NAG:C8	2.44	0.46
1:B:200:TYR:CE2	1:B:230:PRO:HA	2.49	0.46
1:B:417:LYS:O	1:B:421:TYR:CD1	2.68	0.46
1:B:1039:ARG:NE	1:C:1031:GLU:OE1	2.49	0.46
1:A:665:PRO:HB2	1:B:864:LEU:HD21	1.98	0.46
1:B:709:ASN:ND2	5:B:1409:NAG:O5	2.45	0.46
1:A:603:ASN:ND2	5:A:1408:NAG:C2	2.67	0.45
1:A:658:ASN:HB2	1:A:660:TYR:CE2	2.52	0.45
1:B:200:TYR:CD2	1:B:230:PRO:CA	2.97	0.45
1:C:165:ASN:CG	5:C:1404:NAG:C1	2.72	0.45
1:C:722:VAL:H	1:C:930:ALA:HB1	1.82	0.45
1:A:1010:GLN:CB	1:A:1014:ARG:NH1	2.67	0.45
1:B:535:LYS:HE3	1:B:585:LEU:HD11	1.98	0.45
1:B:1116:THR:HA	1:B:1138:TYR:O	2.15	0.45
1:B:1029:MET:HE1	1:B:1053:PRO:HG3	1.98	0.45
1:A:658:ASN:ND2	1:A:660:TYR:OH	2.49	0.45
1:B:403:ARG:HD3	1:B:505:TYR:HA	1.98	0.45
1:B:295:PRO:O	1:B:299:THR:HG23	2.16	0.45
1:C:102:ARG:HE	1:C:141:LEU:HD22	1.81	0.45
1:A:58:PHE:HD1	1:A:290:ASP:HB2	1.82	0.45
1:B:131:CYS:C	1:B:133:PHE:CE2	2.95	0.45
1:C:350:VAL:HG12	1:C:495:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ILE:HD12	1:C:534:VAL:H	1.82	0.44
1:A:796:ASP:CB	5:C:1410:NAG:H82	2.43	0.44
1:B:815:ARG:HG2	1:B:819:GLU:CB	2.47	0.44
1:A:903:ALA:HB2	1:A:917:TYR:HH	1.82	0.44
1:B:436:TRP:HZ2	1:B:509:ARG:HD3	1.79	0.44
1:C:408:ARG:HH12	1:C:411:ALA:HB3	1.81	0.44
1:C:643:PHE:CE1	1:C:655:HIS:CG	3.05	0.44
1:B:913:GLN:HB2	1:B:917:TYR:CE1	2.52	0.44
1:C:64:TRP:CE3	1:C:266:TYR:CE1	3.06	0.44
1:C:1075:PHE:CZ	1:C:1110:TYR:HE1	2.36	0.44
1:A:667:GLY:H	1:B:864:LEU:HD23	1.82	0.44
1:B:357:ARG:NE	1:B:396:TYR:HE2	2.16	0.44
1:C:14:GLN:CD	1:C:158:ARG:NH2	2.70	0.44
1:A:1097:SER:HB2	1:A:1102:TRP:CE3	2.53	0.44
1:C:1010:GLN:O	1:C:1014:ARG:NH1	2.50	0.44
1:A:905:ARG:NH1	1:A:1050:MET:CA	2.80	0.44
1:A:34:ARG:HD2	1:A:217:PRO:O	2.18	0.44
1:A:752:LEU:O	1:A:756:TYR:CD2	2.70	0.44
1:A:896:ILE:CD1	1:A:904:TYR:HE2	2.30	0.44
1:C:452:LEU:HG	1:C:494:SER:HA	1.99	0.44
1:A:318:PHE:HD2	1:A:593:GLY:O	2.01	0.44
1:C:453:TYR:HD1	1:C:495:TYR:CD1	2.35	0.44
1:A:318:PHE:CD2	1:A:318:PHE:C	2.91	0.43
1:A:318:PHE:CD2	1:A:318:PHE:O	2.70	0.43
1:A:273:ARG:CZ	1:A:292:ALA:HB3	2.35	0.43
1:B:44:ARG:CZ	1:B:49:HIS:CD2	3.02	0.43
1:C:452:LEU:HA	1:C:494:SER:HA	2.00	0.43
1:A:17:ASN:HA	1:A:138:ASP:HB2	1.99	0.43
1:B:498:GLN:CD	1:B:501:TYR:CZ	2.95	0.43
1:C:1010:GLN:C	1:C:1014:ARG:HH12	2.27	0.43
2:F:1:NAG:H62	2:F:2:NAG:HN2	1.82	0.43
1:A:34:ARG:O	1:A:56:LEU:HD23	2.18	0.43
1:B:347:PHE:CE1	1:B:509:ARG:NH2	2.84	0.43
1:B:699:LEU:N	1:B:699:LEU:HD12	2.34	0.43
1:C:643:PHE:CZ	1:C:655:HIS:CE1	3.07	0.43
1:C:1075:PHE:CZ	1:C:1110:TYR:CE1	3.07	0.43
1:B:299:THR:HG22	1:B:597:VAL:CG1	2.49	0.43
1:C:408:ARG:NH1	1:C:411:ALA:HB3	2.34	0.43
1:B:877:LEU:HD13	1:B:1029:MET:HE2	2.00	0.43
1:A:1107:ARG:HH11	1:B:904:TYR:HD1	1.67	0.43
1:A:421:TYR:HA	1:A:457:ARG:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:MET:CG	1:C:869:MET:HE1	2.42	0.43
1:C:563:GLN:O	1:C:577:ARG:NE	2.52	0.43
1:B:357:ARG:NH1	1:B:396:TYR:CE2	2.87	0.42
1:A:33:THR:C	1:A:58:PHE:CE2	2.72	0.42
1:B:357:ARG:CD	1:B:396:TYR:CE2	3.02	0.42
1:C:900:MET:HE2	1:C:900:MET:N	2.35	0.42
1:C:125:ASN:CG	1:C:171:VAL:HG13	2.38	0.42
1:A:742:ILE:O	1:A:1000:ARG:HD2	2.18	0.42
1:A:983:ARG:HH11	1:A:984:LEU:HD21	1.84	0.42
1:B:902:MET:O	1:B:905:ARG:HB3	2.19	0.42
1:C:139:PRO:HA	1:C:158:ARG:O	2.19	0.42
1:B:1114:ILE:HD12	1:B:1114:ILE:H	1.84	0.42
1:C:102:ARG:NE	1:C:141:LEU:HD22	2.33	0.42
1:B:905:ARG:CZ	1:B:1050:MET:HB3	2.46	0.42
1:C:987:VAL:O	1:C:991:VAL:HG23	2.20	0.42
1:C:560:LEU:O	1:C:577:ARG:NH2	2.53	0.41
1:A:34:ARG:CZ	1:A:217:PRO:HG2	2.47	0.41
1:A:577:ARG:HH22	1:A:582:LEU:CD2	2.22	0.41
1:A:658:ASN:HB2	1:A:660:TYR:HE2	1.84	0.41
1:B:720:ILE:N	1:B:720:ILE:HD12	2.35	0.41
1:C:44:ARG:NE	1:C:49:HIS:CD2	2.87	0.41
1:C:617:CYS:SG	1:C:644:GLN:NE2	2.92	0.41
1:B:44:ARG:O	1:B:283:GLY:HA2	2.20	0.41
1:B:208:THR:HG23	1:B:210:ILE:HG23	2.01	0.41
1:B:342:PHE:CE2	1:B:368:LEU:HD22	2.54	0.41
1:B:1039:ARG:HB2	1:B:1042:PHE:HB3	2.01	0.41
1:A:34:ARG:NH2	1:A:191:GLU:OE1	2.53	0.41
1:A:902:MET:HG3	1:A:916:LEU:HD22	2.02	0.41
1:C:124:THR:C	1:C:175:PHE:CE2	2.93	0.41
4:J:1:NAG:H5	4:J:2:NAG:C7	2.50	0.41
1:B:90:VAL:HG11	1:B:238:PHE:CE1	2.56	0.41
1:C:1014:ARG:NH1	1:C:1014:ARG:HB2	2.35	0.41
1:B:357:ARG:HD3	1:B:396:TYR:CE2	2.56	0.41
1:C:567:ARG:NH1	1:C:573:THR:N	2.69	0.41
1:A:34:ARG:NH2	1:A:189:LEU:CD2	2.79	0.41
1:A:902:MET:O	1:A:905:ARG:HB2	2.20	0.41
1:C:457:ARG:HH11	1:C:461:LEU:HD23	1.85	0.41
1:C:1011:GLN:OE1	1:C:1014:ARG:NH1	2.54	0.41
1:A:102:ARG:HH11	1:A:179:LEU:CG	2.07	0.41
1:A:37:TYR:CE1	1:A:39:PRO:HA	2.57	0.40
1:A:903:ALA:CB	1:A:917:TYR:CE2	2.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:ARG:NE	1:A:1050:MET:CE	2.80	0.40
1:C:128:ILE:CG1	1:C:170:TYR:HB3	2.52	0.40
1:B:1097:SER:HB2	1:B:1102:TRP:CD1	2.56	0.40
1:C:130:VAL:HG13	1:C:168:PHE:H	1.86	0.40
1:C:1110:TYR:CE2	1:C:1112:PRO:HD3	2.55	0.40
1:A:34:ARG:CZ	1:A:189:LEU:HD21	2.50	0.40
1:B:417:LYS:C	1:B:421:TYR:CE1	2.99	0.40
1:A:102:ARG:NH1	1:A:179:LEU:CG	2.68	0.40
1:C:276:LEU:C	1:C:277:LEU:HD22	2.45	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	1066/1305 (82%)	973 (91%)	86 (8%)	7 (1%)	18	55
1	B	1075/1305 (82%)	971 (90%)	98 (9%)	6 (1%)	21	58
1	C	1065/1305 (82%)	968 (91%)	90 (8%)	7 (1%)	18	55
All	All	3206/3915 (82%)	2912 (91%)	274 (8%)	20 (1%)	23	58

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	316	SER
1	A	316	SER
1	B	709	ASN
1	C	573	THR
1	A	544	ASN
1	A	582	LEU
1	B	132	GLU
1	B	487	ASN

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Mol	Chain	Res	Type
1	C	88	ASP
1	A	985	ASP
1	B	571	ASP
1	C	149	ASN
1	C	368	LEU
1	C	429	PHE
1	B	310	LYS
1	A	163	ALA
1	A	812	PRO
1	A	447	GLY
1	B	410	ILE
1	C	812	PRO

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	942/1130 (83%)	923 (98%)	19 (2%)	48	66
1	B	951/1130 (84%)	935 (98%)	16 (2%)	53	67
1	C	941/1130 (83%)	922 (98%)	19 (2%)	48	66
All	All	2834/3390 (84%)	2780 (98%)	54 (2%)	49	66

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	21	ARG
1	A	90	VAL
1	A	164	ASN
1	A	256	SER
1	A	277	LEU
1	A	298	GLU
1	A	318	PHE
1	A	422	ASN
1	A	588	THR

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Mol	Chain	Res	Type
1	A	595	VAL
1	A	617	CYS
1	A	666	ILE
1	A	675	GLN
1	A	745	ASP
1	A	760	CYS
1	A	773	GLU
1	A	979	ASP
1	A	1113	GLN
1	B	54	LEU
1	B	118	LEU
1	B	120	VAL
1	B	175	PHE
1	B	304	LYS
1	B	376	THR
1	B	406	GLU
1	B	421	TYR
1	B	460	ASN
1	B	617	CYS
1	B	624	ILE
1	B	795	LYS
1	B	884	SER
1	B	935	GLN
1	B	1037	SER
1	B	1150	GLU
1	C	124	THR
1	C	125	ASN
1	C	130	VAL
1	C	169	GLU
1	C	188	ASN
1	C	207	HIS
1	C	228	ASP
1	C	235	ILE
1	C	270	LEU
1	C	296	LEU
1	C	343	ASN
1	C	528	LYS
1	C	617	CYS
1	C	858	LEU
1	C	867	ASP
1	C	874	THR
1	C	1004	LEU

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Mol	Chain	Res	Type
1	C	1029	MET
1	C	1152	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	99	ASN
1	A	121	ASN
1	A	148	ASN
1	A	165	ASN
1	A	173	GLN
1	A	188	ASN
1	A	234	ASN
1	A	354	ASN
1	A	450	ASN
1	A	460	ASN
1	A	536	ASN
1	A	603	ASN
1	A	607	GLN
1	A	658	ASN
1	A	703	ASN
1	A	755	GLN
1	A	804	GLN
1	A	895	GLN
1	A	907	ASN
1	A	949	GLN
1	A	992	GLN
1	A	1054	GLN
1	A	1058	HIS
1	A	1098	ASN
1	A	1101	HIS
1	A	1159	HIS
1	B	52	GLN
1	B	125	ASN
1	B	134	GLN
1	B	149	ASN
1	B	239	GLN
1	B	271	GLN
1	B	343	ASN
1	B	360	ASN
1	B	450	ASN

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Mol	Chain	Res	Type
1	B	709	ASN
1	B	787	GLN
1	B	804	GLN
1	B	872	GLN
1	B	913	GLN
1	B	954	GLN
1	B	969	ASN
1	B	1048	HIS
1	B	1058	HIS
1	C	49	HIS
1	C	81	ASN
1	C	122	ASN
1	C	125	ASN
1	C	165	ASN
1	C	185	ASN
1	C	196	ASN
1	C	239	GLN
1	C	460	ASN
1	C	540	ASN
1	C	544	ASN
1	C	675	GLN
1	C	779	GLN
1	C	804	GLN
1	C	953	ASN
1	C	954	GLN
1	C	955	ASN
1	C	960	ASN
1	C	969	ASN
1	C	1119	ASN
1	C	1125	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

59 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	D	1	1,2	14,14,15	0.67	1 (7%)	17,19,21	0.68	0
2	NAG	D	2	2	14,14,15	1.54	2 (14%)	17,19,21	1.40	3 (17%)
2	NAG	E	1	1,2	14,14,15	1.09	0	17,19,21	0.96	1 (5%)
2	NAG	E	2	2	14,14,15	1.17	2 (14%)	17,19,21	1.10	1 (5%)
2	NAG	F	1	2	14,14,15	0.34	0	17,19,21	0.40	0
2	NAG	F	2	2	14,14,15	1.42	3 (21%)	17,19,21	0.80	0
2	NAG	G	1	1,2	14,14,15	1.36	3 (21%)	17,19,21	0.96	0
2	NAG	G	2	2	14,14,15	1.43	2 (14%)	17,19,21	0.60	0
2	NAG	H	1	1,2	14,14,15	1.41	2 (14%)	17,19,21	1.07	2 (11%)
2	NAG	H	2	2	14,14,15	1.53	2 (14%)	17,19,21	0.91	1 (5%)
3	NAG	I	1	1,3	14,14,15	1.54	4 (28%)	17,19,21	0.76	0
3	NAG	I	2	3	14,14,15	1.47	2 (14%)	17,19,21	1.16	1 (5%)
3	FUC	I	3	3	10,10,11	1.15	0	14,14,16	0.95	1 (7%)
4	NAG	J	1	4	14,14,15	0.91	1 (7%)	17,19,21	1.12	2 (11%)
4	NAG	J	2	4	14,14,15	1.33	2 (14%)	17,19,21	1.00	1 (5%)
4	MAN	J	3	4	11,11,12	1.50	2 (18%)	15,15,17	0.92	1 (6%)
4	NAG	K	1	4,1	14,14,15	1.08	1 (7%)	17,19,21	1.04	1 (5%)
4	NAG	K	2	4	14,14,15	1.12	1 (7%)	17,19,21	1.20	1 (5%)
4	MAN	K	3	4	11,11,12	1.48	2 (18%)	15,15,17	1.04	1 (6%)
2	NAG	L	1	1,2	14,14,15	0.39	0	17,19,21	0.66	0
2	NAG	L	2	2	14,14,15	1.37	1 (7%)	17,19,21	1.10	2 (11%)
2	NAG	M	1	1,2	14,14,15	1.21	1 (7%)	17,19,21	1.23	3 (17%)
2	NAG	M	2	2	14,14,15	1.42	1 (7%)	17,19,21	0.82	0
2	NAG	N	1	1,2	14,14,15	1.21	0	17,19,21	1.80	5 (29%)
2	NAG	N	2	2	14,14,15	1.35	2 (14%)	17,19,21	1.20	2 (11%)
2	NAG	O	1	1,2	14,14,15	1.23	1 (7%)	17,19,21	1.56	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	O	2	2	14,14,15	1.43	3 (21%)	17,19,21	0.85	1 (5%)
2	NAG	P	1	1,2	14,14,15	1.08	1 (7%)	17,19,21	0.84	0
2	NAG	P	2	2	14,14,15	1.44	3 (21%)	17,19,21	0.82	0
2	NAG	Q	1	1,2	14,14,15	1.32	2 (14%)	17,19,21	1.12	2 (11%)
2	NAG	Q	2	2	14,14,15	1.30	3 (21%)	17,19,21	1.17	1 (5%)
3	NAG	R	1	1,3	14,14,15	1.95	5 (35%)	17,19,21	1.01	0
3	NAG	R	2	3	14,14,15	1.43	2 (14%)	17,19,21	0.78	0
3	FUC	R	3	3	10,10,11	1.65	2 (20%)	14,14,16	1.05	0
4	NAG	S	1	4,1	14,14,15	1.09	1 (7%)	17,19,21	1.20	1 (5%)
4	NAG	S	2	4	14,14,15	1.73	5 (35%)	17,19,21	0.71	0
4	MAN	S	3	4	11,11,12	1.28	1 (9%)	15,15,17	1.05	1 (6%)
4	NAG	T	1	4,1	14,14,15	1.42	4 (28%)	17,19,21	0.97	1 (5%)
4	NAG	T	2	4	14,14,15	1.47	2 (14%)	17,19,21	0.76	0
4	MAN	T	3	4	11,11,12	1.39	2 (18%)	15,15,17	1.55	2 (13%)
2	NAG	U	1	1,2	14,14,15	0.37	0	17,19,21	0.36	0
2	NAG	U	2	2	14,14,15	1.23	2 (14%)	17,19,21	0.99	0
2	NAG	V	1	1,2	14,14,15	1.48	3 (21%)	17,19,21	1.66	5 (29%)
2	NAG	V	2	2	14,14,15	1.61	4 (28%)	17,19,21	1.64	1 (5%)
2	NAG	W	1	2	14,14,15	0.74	1 (7%)	17,19,21	0.61	0
2	NAG	W	2	2	14,14,15	1.04	1 (7%)	17,19,21	1.00	1 (5%)
2	NAG	X	1	1,2	14,14,15	1.30	2 (14%)	17,19,21	1.10	1 (5%)
2	NAG	X	2	2	14,14,15	1.40	2 (14%)	17,19,21	0.68	0
2	NAG	Y	1	1,2	14,14,15	1.27	2 (14%)	17,19,21	1.13	2 (11%)
2	NAG	Y	2	2	14,14,15	1.07	0	17,19,21	1.59	3 (17%)
3	NAG	Z	1	1,3	14,14,15	1.53	4 (28%)	17,19,21	1.17	1 (5%)
3	NAG	Z	2	3	14,14,15	1.16	2 (14%)	17,19,21	1.03	1 (5%)
3	FUC	Z	3	3	10,10,11	1.75	3 (30%)	14,14,16	1.75	2 (14%)
4	NAG	a	1	4,1	14,14,15	1.15	2 (14%)	17,19,21	1.13	2 (11%)
4	NAG	a	2	4	14,14,15	1.22	2 (14%)	17,19,21	0.99	1 (5%)
4	MAN	a	3	4	11,11,12	1.50	2 (18%)	15,15,17	1.28	2 (13%)
4	NAG	b	1	4,1	14,14,15	1.51	2 (14%)	17,19,21	1.28	2 (11%)
4	NAG	b	2	4	14,14,15	1.27	1 (7%)	17,19,21	1.06	1 (5%)
4	MAN	b	3	4	11,11,12	1.60	2 (18%)	15,15,17	0.98	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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	2	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	FUC	I	3	3	-	-	0/1/1/1
4	NAG	J	1	4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	MAN	J	3	4	-	1/2/19/22	1/1/1/1
4	NAG	K	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	MAN	K	3	4	-	0/2/19/22	1/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	O	2	2	-	1/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	FUC	R	3	3	-	-	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	MAN	S	3	4	-	1/2/19/22	1/1/1/1
4	NAG	T	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	T	3	4	-	0/2/19/22	1/1/1/1
2	NAG	U	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	U	2	2	-	2/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	1/6/23/26	0/1/1/1
2	NAG	W	1	2	-	2/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	1/6/23/26	0/1/1/1
2	NAG	Y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	0/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
3	FUC	Z	3	3	-	-	0/1/1/1
4	NAG	a	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	MAN	a	3	4	-	2/2/19/22	1/1/1/1
4	NAG	b	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	MAN	b	3	4	-	0/2/19/22	1/1/1/1

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	O5-C5	4.71	1.52	1.43
2	L	2	NAG	O5-C5	4.17	1.51	1.43
2	F	2	NAG	O5-C5	3.84	1.50	1.43
3	R	1	NAG	C1-C2	3.57	1.57	1.52
4	b	3	MAN	O5-C5	3.54	1.50	1.43
3	I	2	NAG	O5-C5	3.53	1.50	1.43
3	R	2	NAG	C1-C2	3.52	1.57	1.52
4	K	3	MAN	O5-C5	3.52	1.50	1.43
2	X	2	NAG	O5-C5	3.50	1.50	1.43
3	R	1	NAG	O5-C5	3.44	1.50	1.43
4	K	1	NAG	O5-C1	-3.42	1.37	1.43
4	S	2	NAG	O5-C1	3.40	1.49	1.43
3	R	3	FUC	O5-C5	3.32	1.50	1.43
2	Y	1	NAG	O5-C5	3.31	1.49	1.43
3	Z	1	NAG	O5-C5	3.29	1.49	1.43
2	G	2	NAG	C1-C2	3.28	1.56	1.52
4	b	1	NAG	C1-C2	3.20	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	1	NAG	O5-C5	3.10	1.49	1.43
2	V	2	NAG	O5-C1	3.09	1.48	1.43
2	Q	1	NAG	O5-C5	3.09	1.49	1.43
2	N	2	NAG	O5-C1	3.04	1.48	1.43
3	Z	3	FUC	O5-C5	3.03	1.49	1.43
3	I	1	NAG	C1-C2	3.01	1.56	1.52
3	R	1	NAG	C8-C7	3.00	1.56	1.50
4	S	2	NAG	O5-C5	2.99	1.49	1.43
2	O	2	NAG	C1-C2	2.98	1.56	1.52
2	X	1	NAG	O5-C5	2.97	1.49	1.43
2	H	1	NAG	O5-C5	2.95	1.49	1.43
2	M	1	NAG	O5-C5	2.94	1.49	1.43
2	H	1	NAG	C1-C2	2.94	1.56	1.52
2	M	2	NAG	O5-C5	2.92	1.49	1.43
3	I	2	NAG	C8-C7	2.91	1.56	1.50
2	P	1	NAG	O5-C5	2.88	1.49	1.43
4	b	1	NAG	O5-C1	2.87	1.48	1.43
3	R	1	NAG	O5-C1	2.86	1.48	1.43
2	H	2	NAG	O5-C1	2.84	1.48	1.43
4	J	1	NAG	O5-C1	-2.82	1.39	1.43
4	J	2	NAG	O5-C5	2.81	1.48	1.43
2	V	1	NAG	C1-C2	2.81	1.56	1.52
4	T	3	MAN	O5-C1	2.81	1.48	1.43
4	T	3	MAN	O5-C5	2.80	1.48	1.43
2	N	2	NAG	O5-C5	2.80	1.48	1.43
4	T	2	NAG	O5-C5	2.78	1.48	1.43
3	Z	2	NAG	O5-C5	2.75	1.48	1.43
4	T	1	NAG	O5-C5	2.74	1.48	1.43
2	V	2	NAG	C8-C7	2.73	1.56	1.50
3	Z	3	FUC	O5-C1	2.72	1.48	1.43
2	W	2	NAG	O5-C5	2.72	1.48	1.43
4	a	3	MAN	O5-C1	2.71	1.48	1.43
2	U	2	NAG	O5-C5	2.69	1.48	1.43
3	Z	1	NAG	O5-C1	2.66	1.48	1.43
2	U	2	NAG	C8-C7	2.66	1.56	1.50
2	X	1	NAG	C1-C2	2.64	1.55	1.52
4	a	3	MAN	O5-C5	2.64	1.48	1.43
3	R	1	NAG	O4-C4	2.59	1.49	1.43
4	J	3	MAN	O5-C1	2.54	1.48	1.43
2	W	1	NAG	O5-C1	-2.51	1.39	1.43
4	a	1	NAG	O5-C5	2.51	1.48	1.43
4	T	2	NAG	O5-C1	2.51	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	O5-C1	2.50	1.47	1.43
2	O	2	NAG	O5-C1	2.50	1.47	1.43
3	Z	2	NAG	O5-C1	2.49	1.47	1.43
2	Q	2	NAG	O5-C5	2.46	1.48	1.43
3	I	1	NAG	O5-C5	2.45	1.48	1.43
2	P	2	NAG	O5-C5	2.43	1.48	1.43
3	Z	1	NAG	C1-C2	2.41	1.55	1.52
4	K	2	NAG	O5-C5	2.40	1.48	1.43
4	S	2	NAG	C1-C2	2.38	1.55	1.52
2	G	1	NAG	O5-C5	2.37	1.48	1.43
3	I	1	NAG	C8-C7	2.35	1.55	1.50
4	b	2	NAG	O5-C1	2.34	1.47	1.43
2	Q	2	NAG	C8-C7	2.34	1.55	1.50
2	D	2	NAG	C8-C7	2.34	1.55	1.50
2	O	1	NAG	O4-C4	2.33	1.48	1.43
4	S	2	NAG	O4-C4	2.33	1.48	1.43
3	R	3	FUC	O5-C1	2.30	1.47	1.43
2	X	2	NAG	O5-C1	2.29	1.47	1.43
2	D	1	NAG	O5-C1	-2.29	1.39	1.43
3	Z	3	FUC	C2-C3	2.26	1.56	1.52
2	V	1	NAG	O4-C4	2.25	1.48	1.43
4	a	2	NAG	O4-C4	2.25	1.48	1.43
2	P	2	NAG	C8-C7	2.25	1.55	1.50
4	J	2	NAG	O4-C4	2.24	1.48	1.43
4	T	1	NAG	C1-C2	2.23	1.55	1.52
2	G	2	NAG	O5-C5	2.23	1.47	1.43
2	Q	1	NAG	O5-C1	2.22	1.47	1.43
4	J	3	MAN	O5-C5	2.20	1.47	1.43
4	S	3	MAN	O5-C1	2.20	1.47	1.43
4	a	1	NAG	C1-C2	2.20	1.55	1.52
3	Z	1	NAG	C8-C7	2.18	1.55	1.50
2	P	2	NAG	C1-C2	2.18	1.55	1.52
3	R	2	NAG	O5-C5	2.17	1.47	1.43
4	T	1	NAG	C8-C7	2.17	1.55	1.50
3	I	1	NAG	O5-C1	2.17	1.47	1.43
2	Y	1	NAG	C8-C7	2.15	1.55	1.50
2	G	1	NAG	C1-C2	2.15	1.55	1.52
4	b	3	MAN	O3-C3	2.14	1.48	1.43
2	F	2	NAG	C8-C7	2.14	1.55	1.50
2	Q	2	NAG	C1-C2	2.13	1.55	1.52
2	V	2	NAG	C1-C2	2.12	1.55	1.52
4	T	1	NAG	O4-C4	2.11	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	2	NAG	O5-C5	2.11	1.47	1.43
4	K	3	MAN	O5-C1	2.10	1.47	1.43
4	a	2	NAG	O5-C5	2.09	1.47	1.43
2	H	2	NAG	C8-C7	2.07	1.54	1.50
4	S	2	NAG	C8-C7	2.06	1.54	1.50
2	G	1	NAG	C8-C7	2.05	1.54	1.50
2	O	2	NAG	O5-C5	2.04	1.47	1.43
2	E	2	NAG	O5-C5	2.03	1.47	1.43
2	F	2	NAG	O3-C3	2.01	1.47	1.43
4	S	1	NAG	O4-C4	2.01	1.47	1.43

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	2	NAG	C1-O5-C5	6.27	120.59	112.19
4	T	3	MAN	C1-O5-C5	4.85	118.69	112.19
2	Y	2	NAG	C1-O5-C5	4.44	118.14	112.19
4	S	1	NAG	C1-O5-C5	4.36	118.04	112.19
2	O	1	NAG	C4-C3-C2	4.34	117.38	111.02
2	N	1	NAG	C3-C4-C5	4.14	117.74	110.23
3	Z	3	FUC	C1-C2-C3	4.04	115.52	109.64
2	Q	2	NAG	O5-C1-C2	-3.78	105.45	111.29
3	Z	3	FUC	C1-O5-C5	3.75	121.81	112.97
4	K	2	NAG	C1-O5-C5	3.66	117.09	112.19
4	a	3	MAN	O3-C3-C2	-3.60	102.70	110.05
2	V	1	NAG	C1-O5-C5	3.58	116.98	112.19
3	Z	1	NAG	C1-O5-C5	3.56	116.96	112.19
4	b	1	NAG	O5-C1-C2	-3.37	106.08	111.29
2	V	1	NAG	C4-C3-C2	3.20	115.70	111.02
4	a	1	NAG	C3-C4-C5	3.09	115.83	110.23
4	a	2	NAG	O4-C4-C5	-3.05	101.80	109.32
2	D	2	NAG	C1-O5-C5	3.03	116.25	112.19
4	K	3	MAN	C1-O5-C5	3.01	116.22	112.19
4	K	1	NAG	C3-C4-C5	2.90	115.49	110.23
4	J	3	MAN	C1-O5-C5	2.89	116.06	112.19
2	Y	2	NAG	O5-C1-C2	-2.85	106.89	111.29
3	I	2	NAG	C1-O5-C5	2.83	115.98	112.19
2	V	1	NAG	O4-C4-C3	-2.82	103.72	110.38
2	O	1	NAG	C3-C4-C5	2.81	115.32	110.23
2	M	1	NAG	O5-C1-C2	-2.78	106.99	111.29
2	Y	1	NAG	C1-O5-C5	2.77	115.90	112.19
2	E	1	NAG	C1-O5-C5	2.77	115.90	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	2	NAG	C4-C3-C2	-2.77	106.96	111.02
2	N	1	NAG	C4-C3-C2	2.74	115.03	111.02
4	b	1	NAG	C3-C4-C5	2.72	115.16	110.23
4	a	3	MAN	C1-O5-C5	2.66	115.75	112.19
2	Y	1	NAG	C4-C3-C2	-2.65	107.14	111.02
2	E	2	NAG	C1-O5-C5	2.53	115.57	112.19
4	J	2	NAG	C1-O5-C5	2.52	115.56	112.19
4	J	1	NAG	C3-C4-C5	2.51	114.78	110.23
2	X	1	NAG	O3-C3-C2	2.51	114.61	109.40
2	L	2	NAG	C1-O5-C5	2.51	115.55	112.19
2	V	1	NAG	C3-C4-C5	2.47	114.70	110.23
2	D	2	NAG	C4-C3-C2	-2.43	107.45	111.02
2	N	1	NAG	O4-C4-C3	-2.37	104.80	110.38
3	I	3	FUC	C6-C5-C4	2.30	117.29	113.08
2	V	1	NAG	O5-C1-C2	-2.30	107.74	111.29
3	Z	2	NAG	O4-C4-C3	-2.28	105.00	110.38
2	H	2	NAG	C3-C4-C5	2.27	114.34	110.23
4	T	3	MAN	C1-C2-C3	2.26	112.94	109.64
2	W	2	NAG	O4-C4-C3	-2.26	105.06	110.38
2	H	1	NAG	C3-C4-C5	2.25	114.31	110.23
2	M	1	NAG	O4-C4-C5	-2.21	103.89	109.32
2	Y	2	NAG	C4-C3-C2	-2.19	107.81	111.02
4	J	1	NAG	C1-O5-C5	2.18	115.11	112.19
4	b	3	MAN	O5-C5-C6	2.16	111.86	107.66
2	D	2	NAG	O5-C5-C6	2.14	111.83	107.66
4	S	3	MAN	C1-O5-C5	2.14	115.05	112.19
2	Q	1	NAG	O5-C1-C2	-2.13	107.99	111.29
2	Q	1	NAG	O4-C4-C3	-2.13	105.36	110.38
4	T	1	NAG	C1-O5-C5	2.12	115.03	112.19
2	O	1	NAG	C2-N2-C7	2.09	125.70	122.90
2	N	1	NAG	O4-C4-C5	-2.09	104.18	109.32
4	a	1	NAG	O4-C4-C3	-2.08	105.47	110.38
2	N	1	NAG	O5-C5-C6	2.07	111.69	107.66
2	O	1	NAG	C1-C2-N2	-2.07	107.17	110.43
2	H	1	NAG	O5-C1-C2	-2.07	108.09	111.29
2	L	2	NAG	C2-N2-C7	2.05	125.64	122.90
2	M	1	NAG	C4-C3-C2	-2.04	108.02	111.02
2	N	2	NAG	O5-C1-C2	-2.03	108.15	111.29
2	O	2	NAG	C2-N2-C7	2.02	125.61	122.90
4	b	2	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	Z	1	NAG	O5-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	Z	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
4	S	3	MAN	O5-C5-C6-O6
4	a	3	MAN	O5-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	J	3	MAN	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	U	2	NAG	C3-C2-N2-C7
2	X	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C1-C2-N2-C7
2	O	2	NAG	C1-C2-N2-C7
2	P	2	NAG	C1-C2-N2-C7
2	U	2	NAG	C1-C2-N2-C7
3	I	2	NAG	C1-C2-N2-C7
2	O	1	NAG	C3-C2-N2-C7
2	W	1	NAG	C4-C5-C6-O6
4	a	3	MAN	C4-C5-C6-O6

All (6) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	S	3	MAN	C1-C2-C3-C4-C5-O5
4	b	3	MAN	C1-C2-C3-C4-C5-O5
4	a	3	MAN	C1-C2-C3-C4-C5-O5

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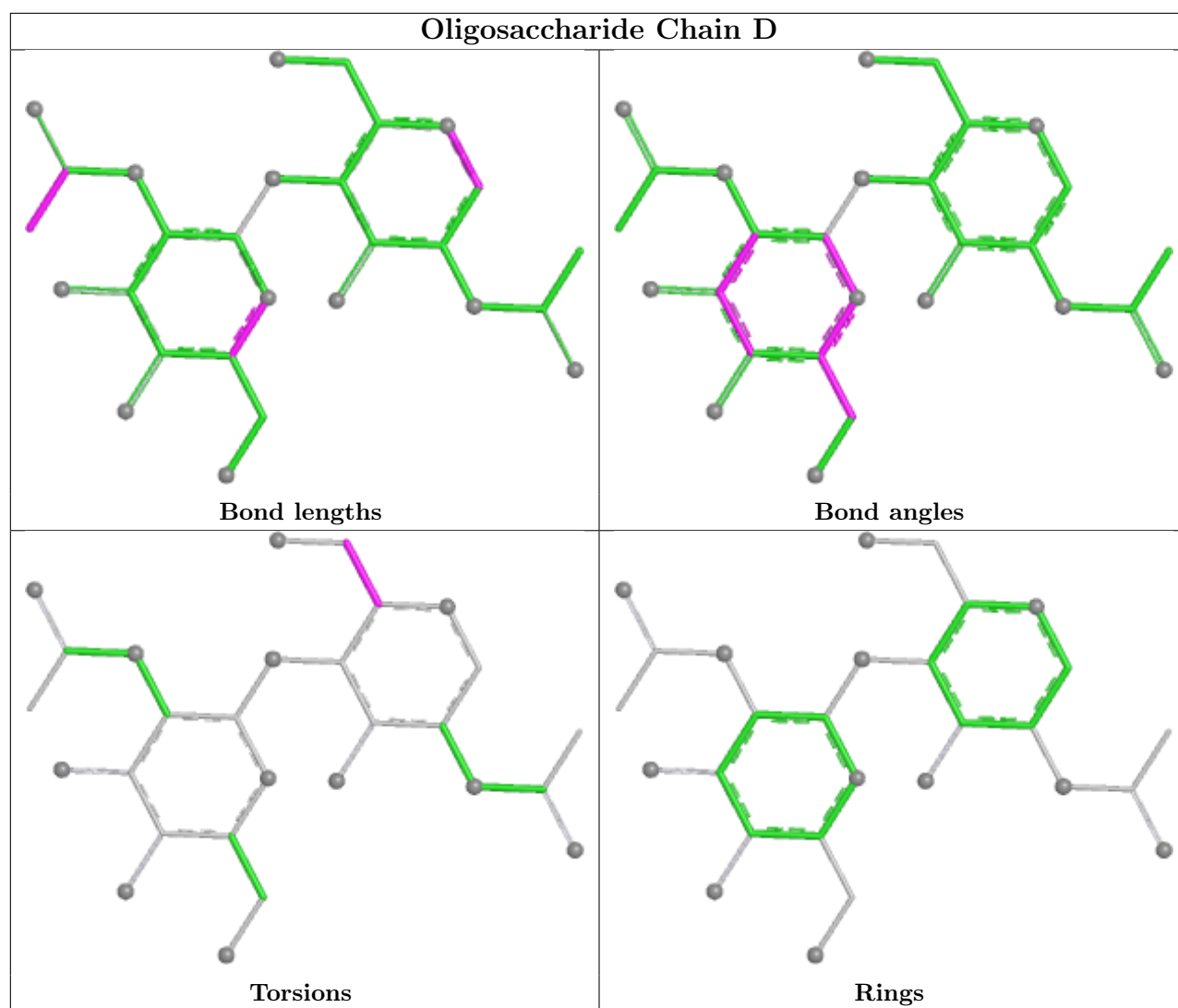
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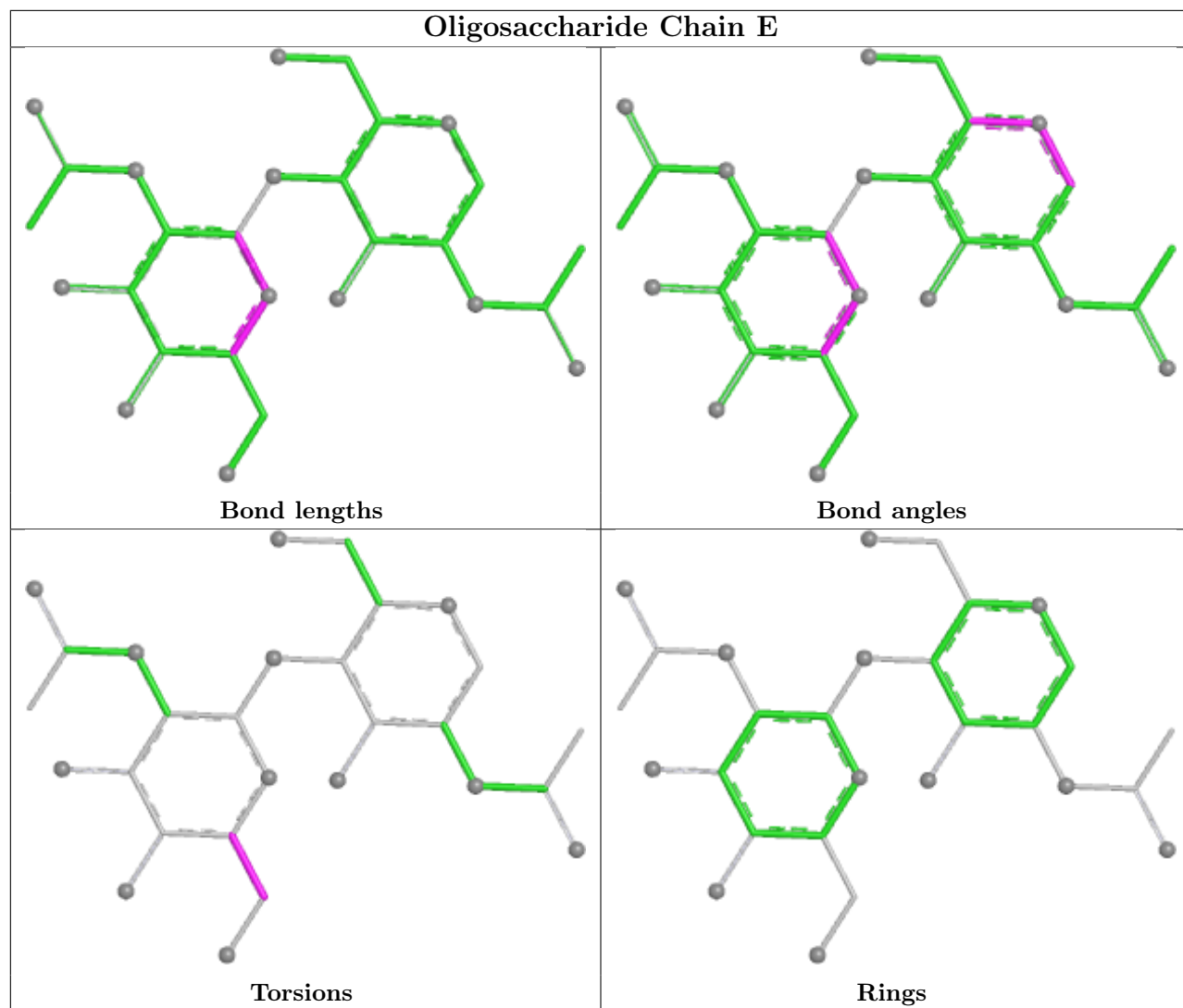
Mol	Chain	Res	Type	Atoms
4	J	3	MAN	C1-C2-C3-C4-C5-O5
4	T	3	MAN	C1-C2-C3-C4-C5-O5
4	K	3	MAN	C1-C2-C3-C4-C5-O5

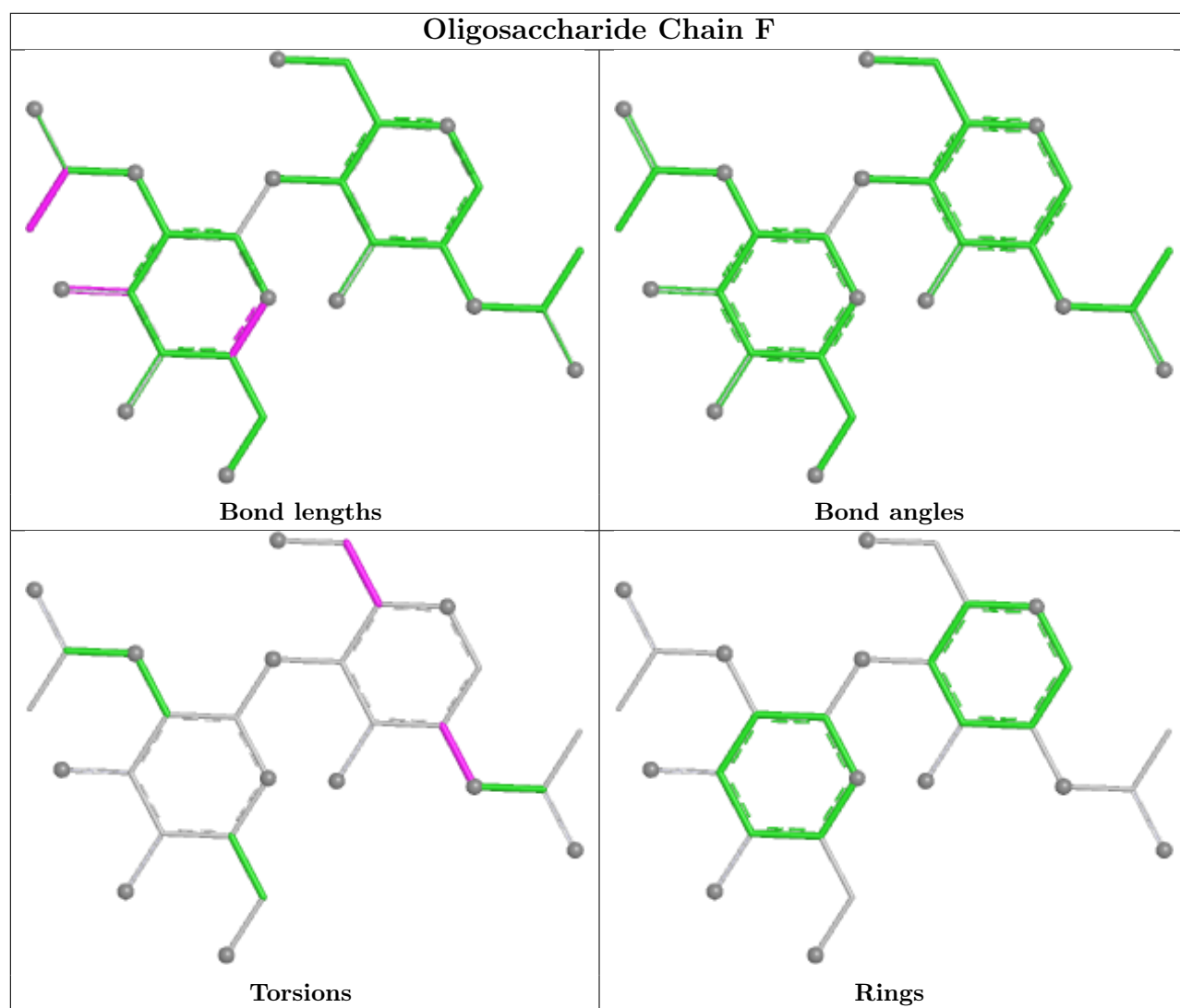
12 monomers are involved in 20 short contacts:

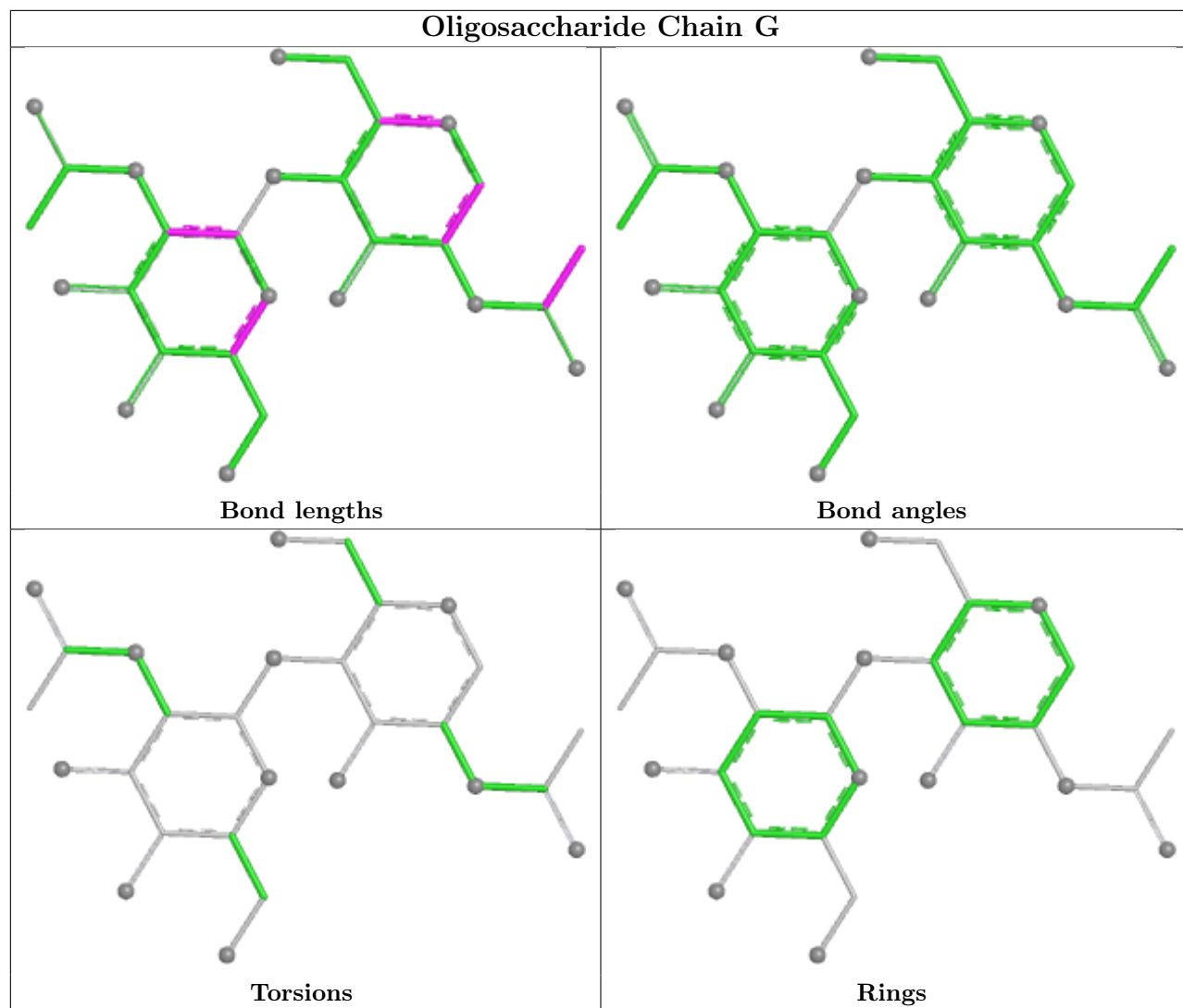
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	U	2	NAG	1	0
2	W	2	NAG	4	0
2	L	1	NAG	1	0
2	L	2	NAG	1	0
2	F	1	NAG	5	0
4	J	2	NAG	1	0
2	D	2	NAG	1	0
4	J	1	NAG	6	0
2	F	2	NAG	1	0
2	W	1	NAG	6	0
2	D	1	NAG	1	0
2	U	1	NAG	1	0

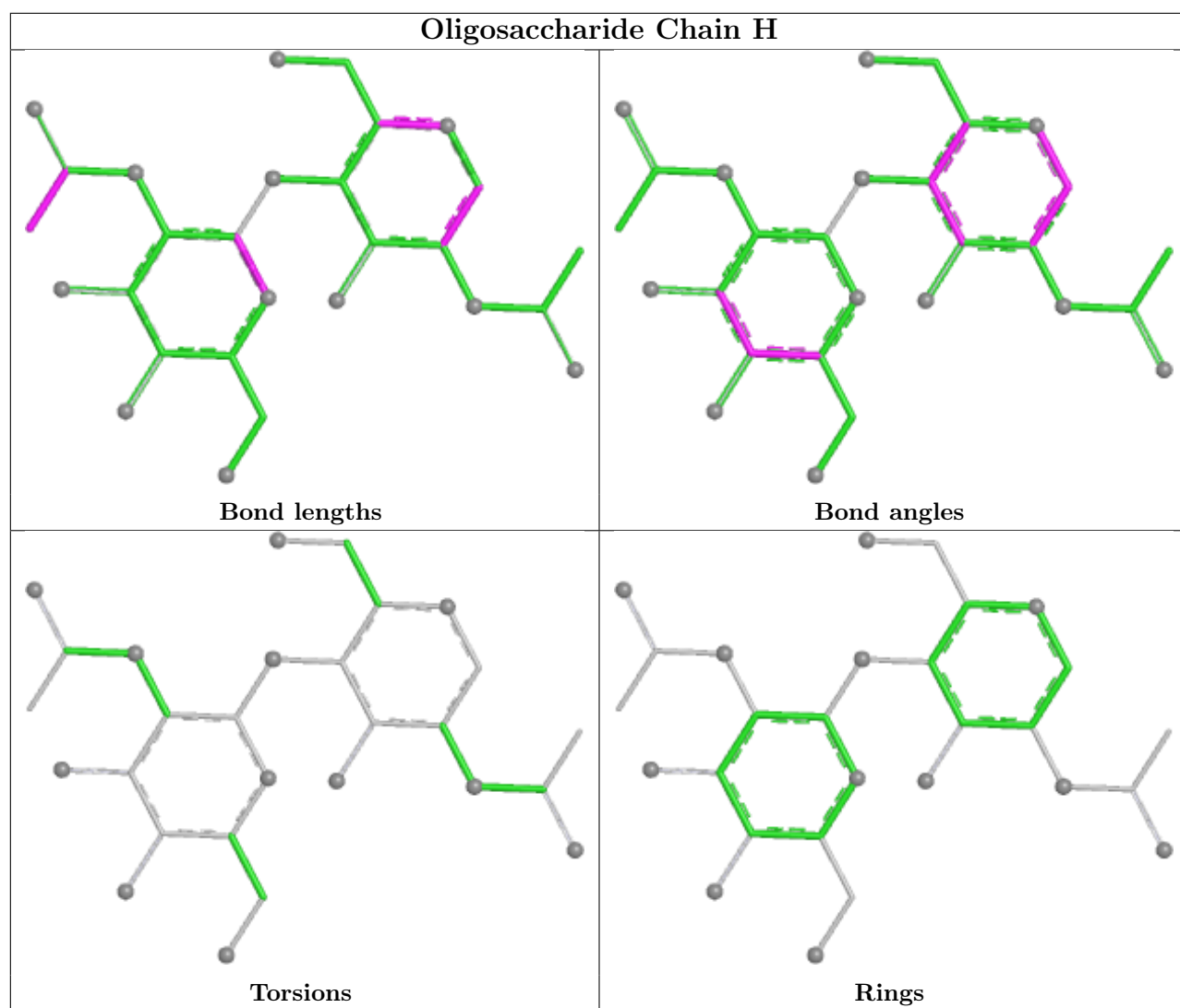
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

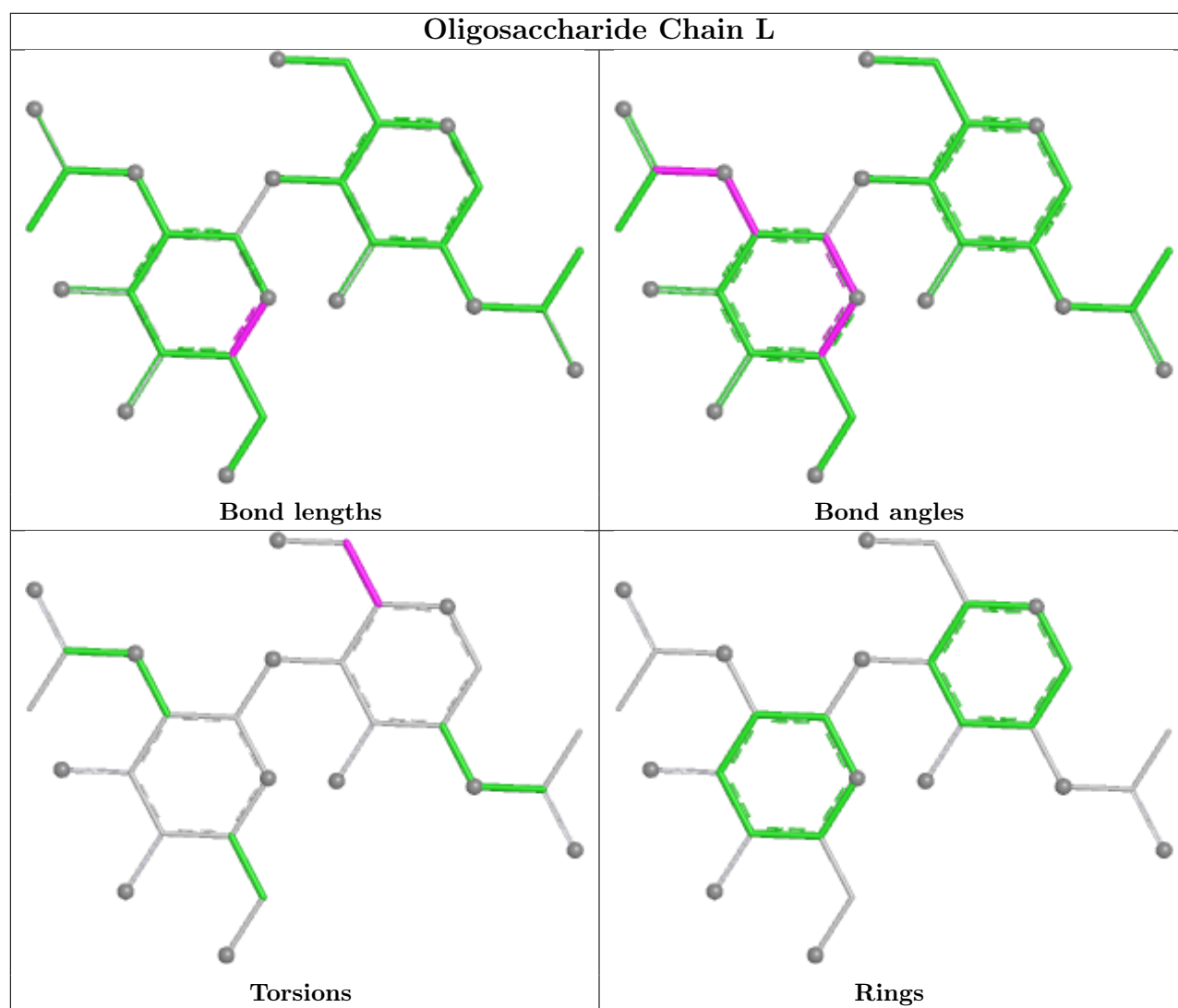


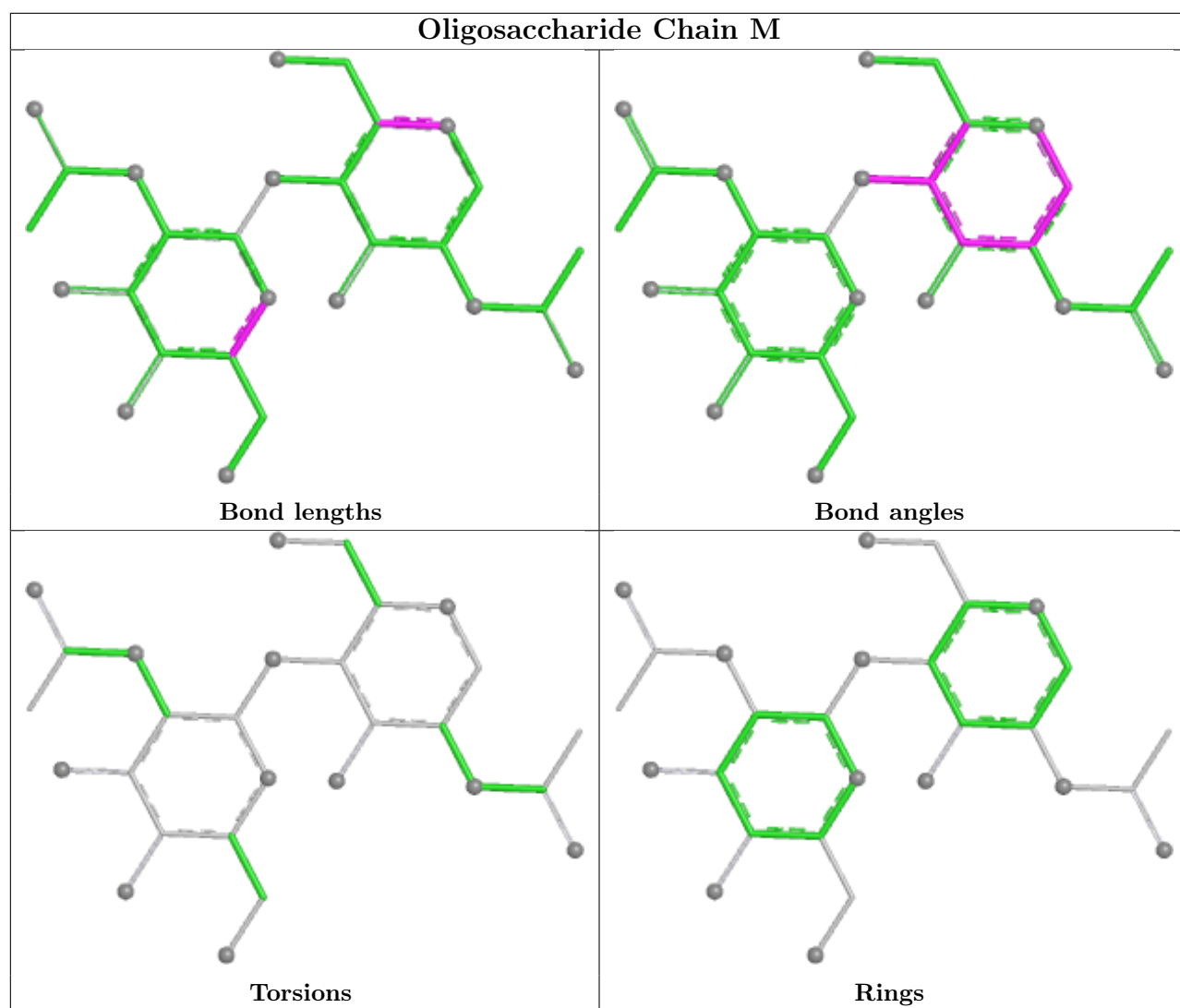


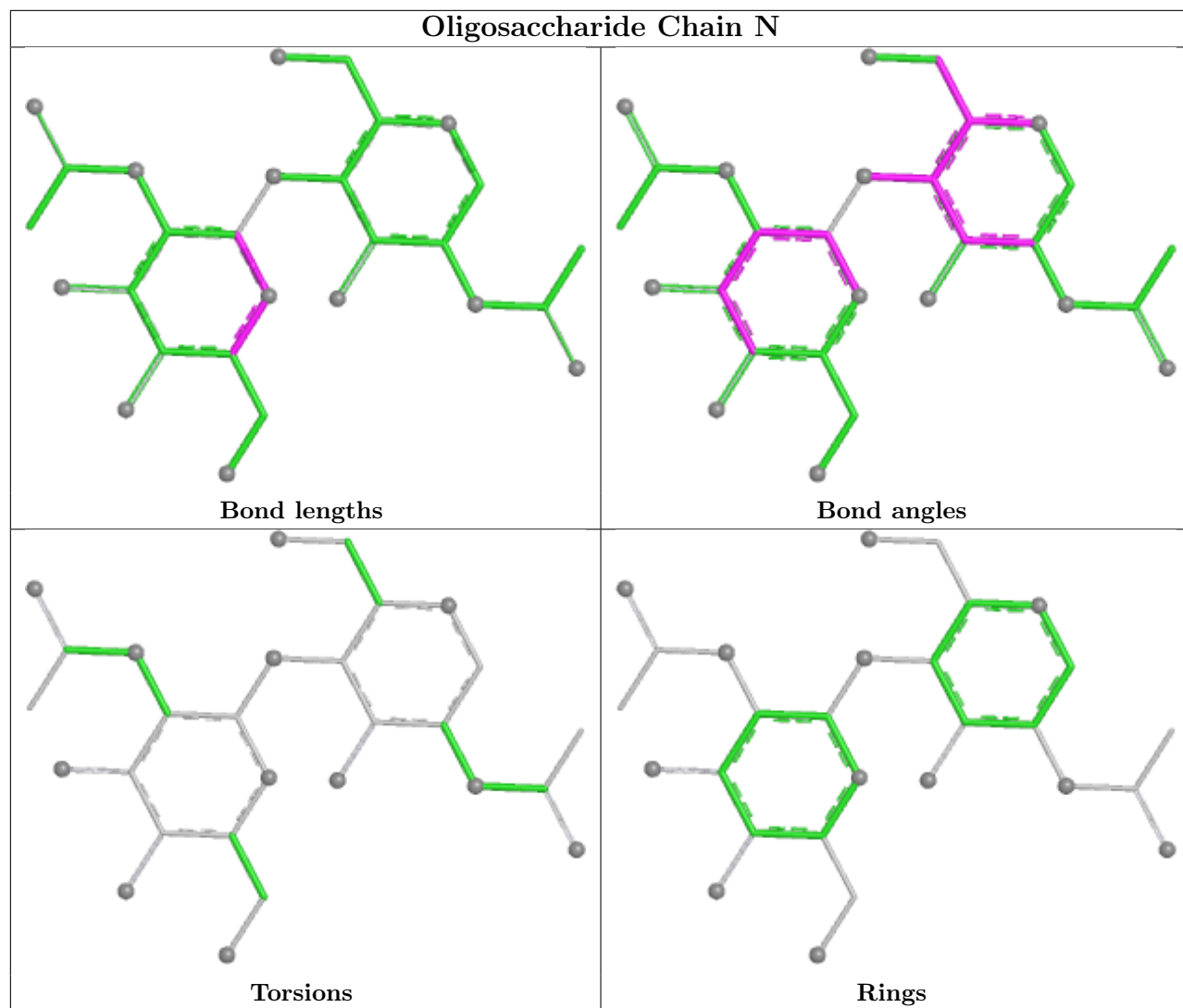


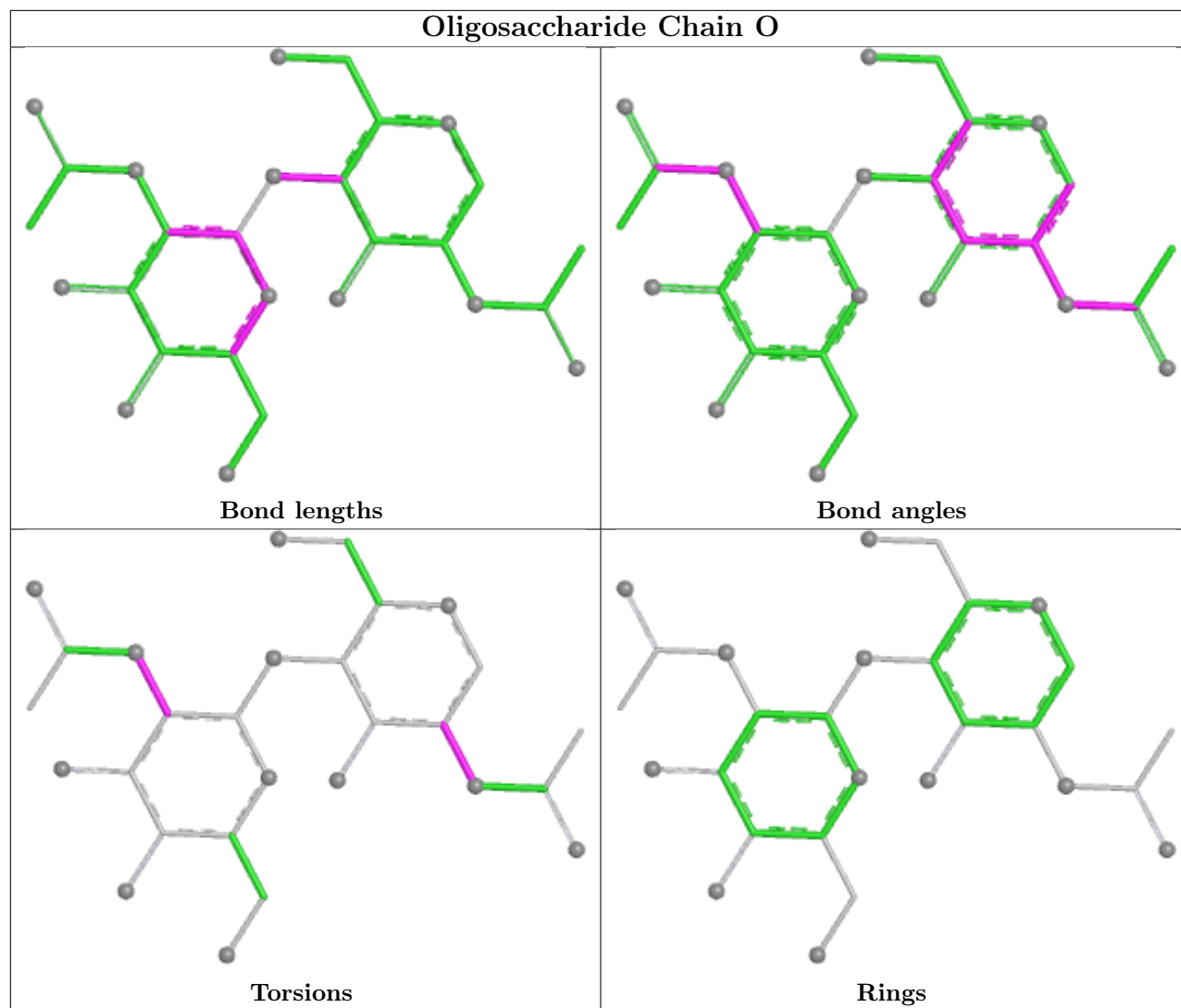


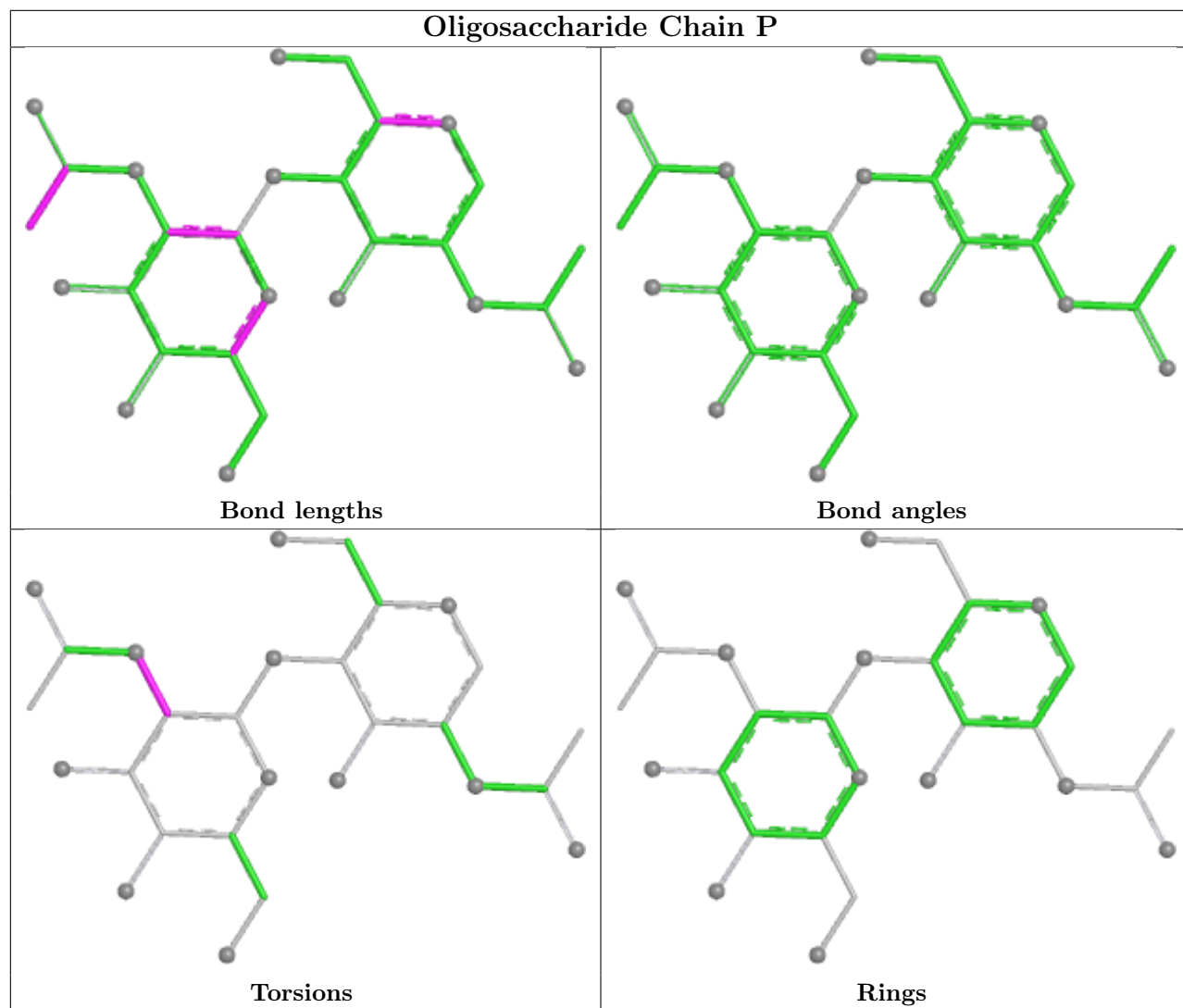


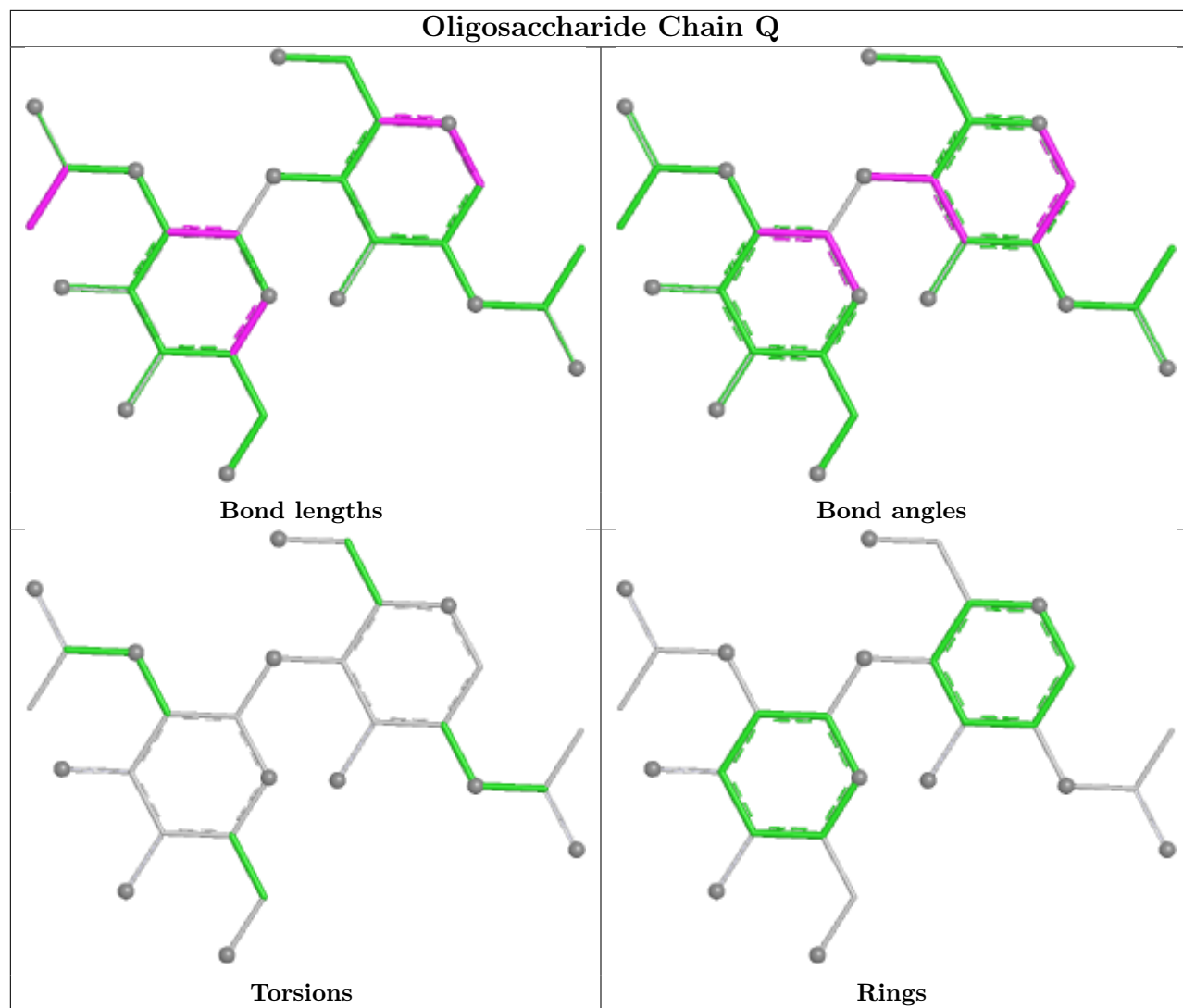


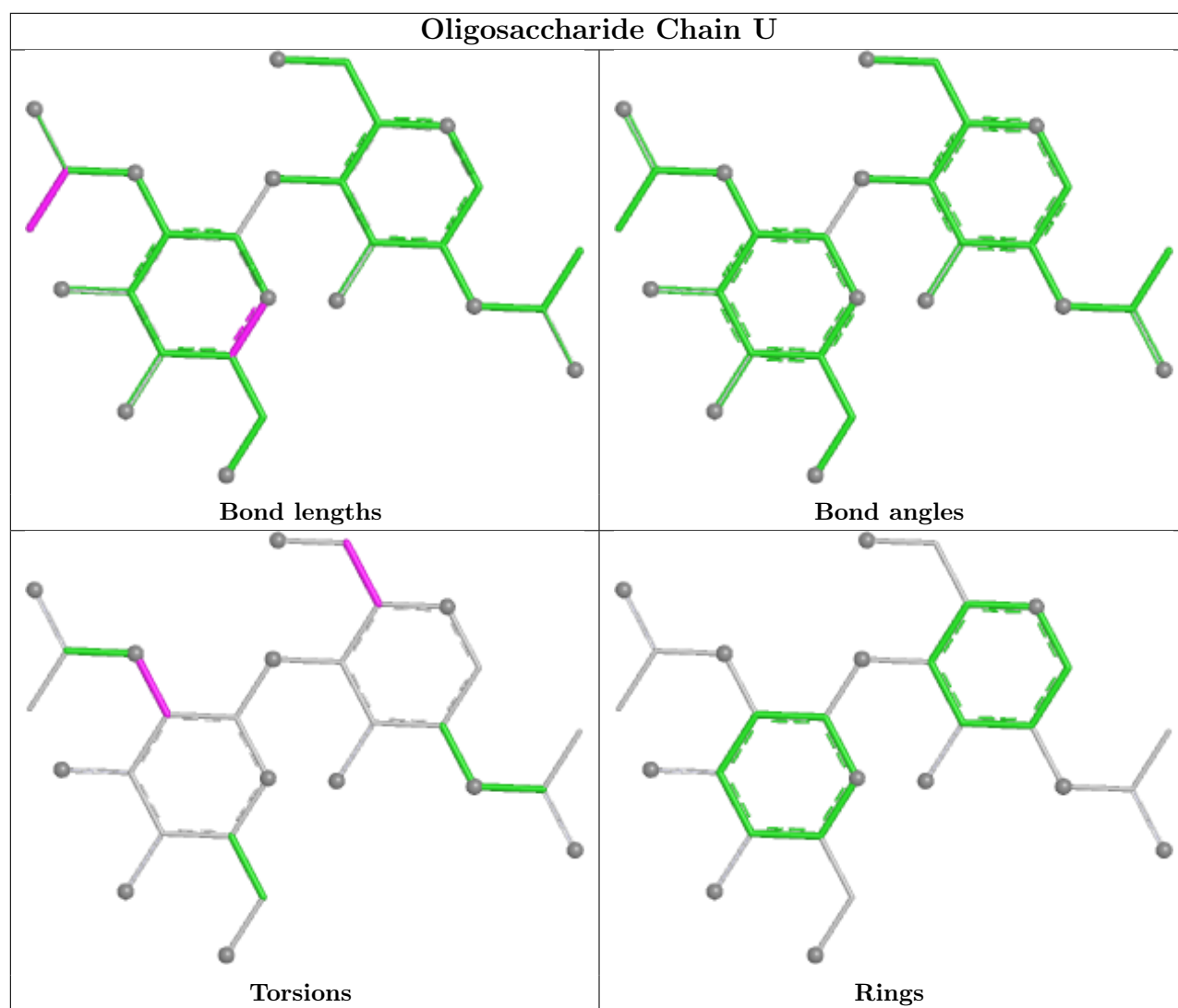


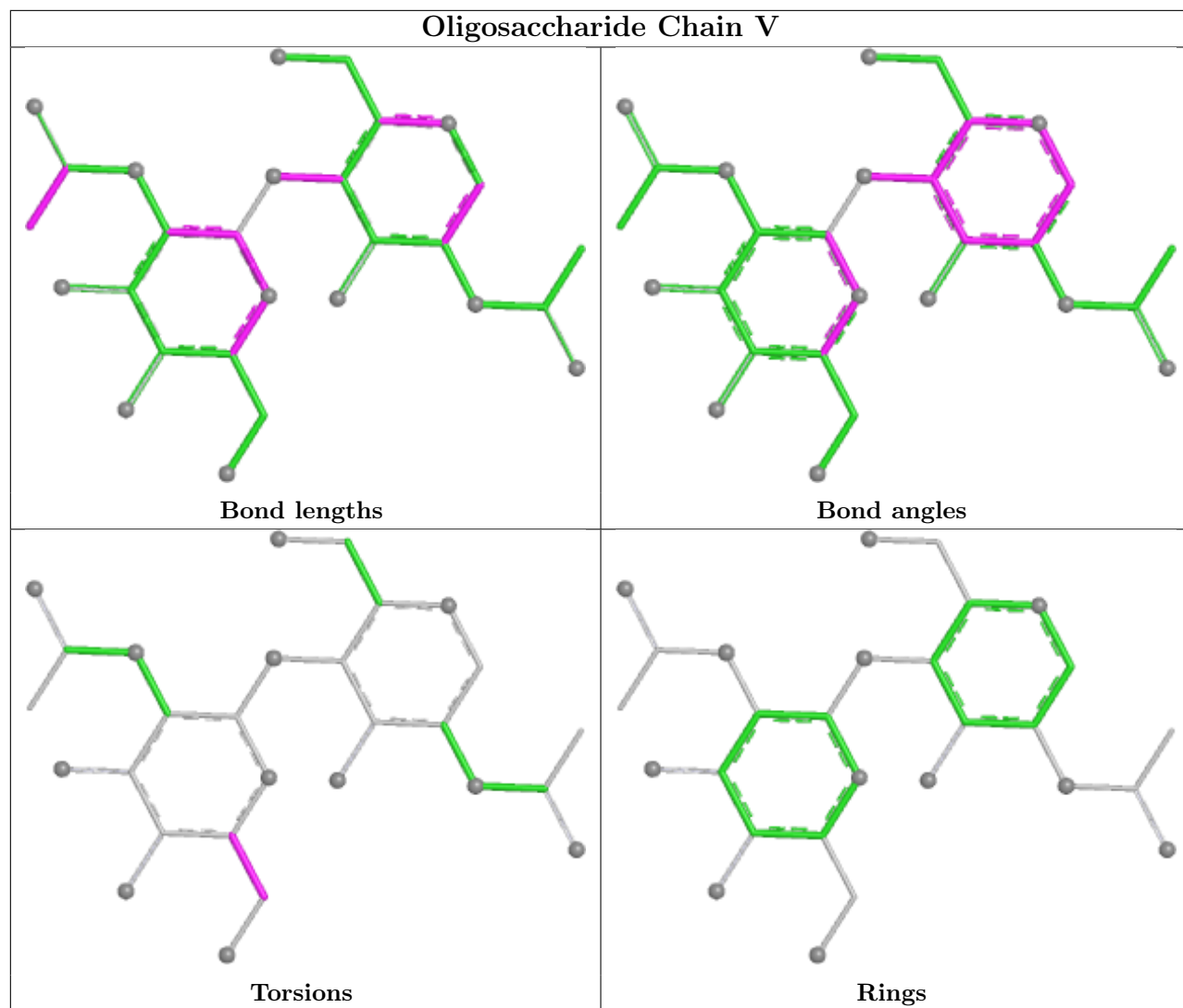


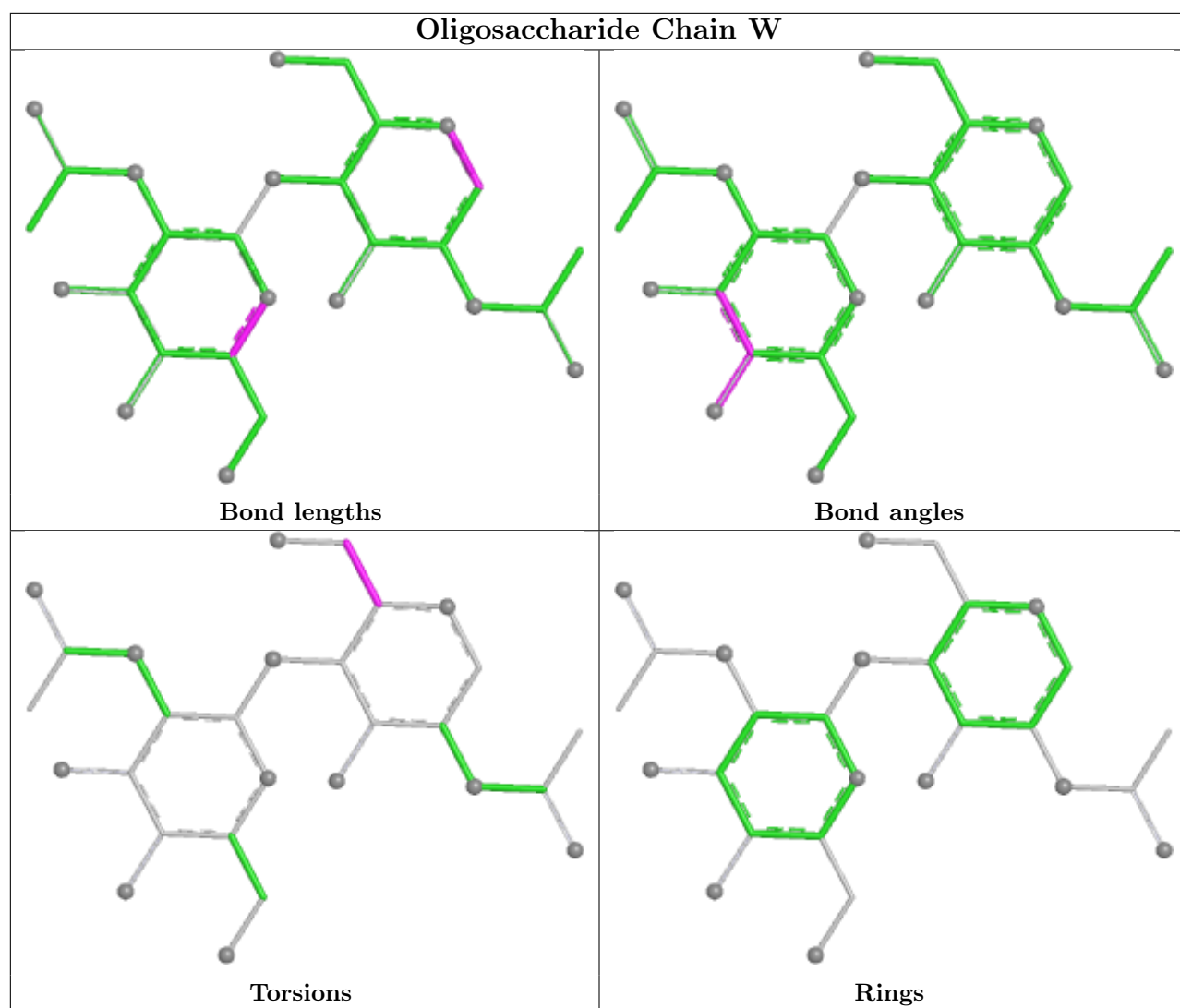


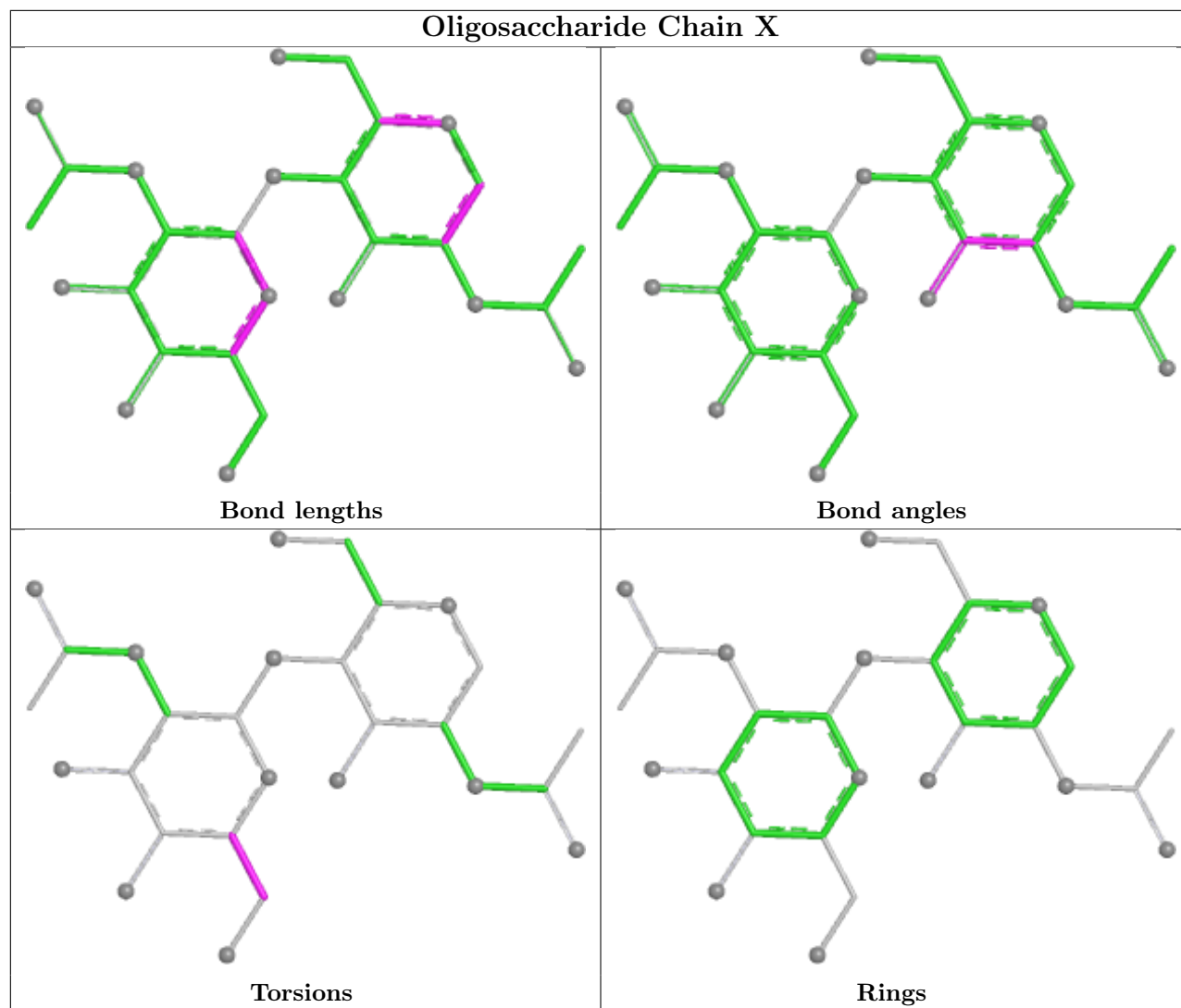


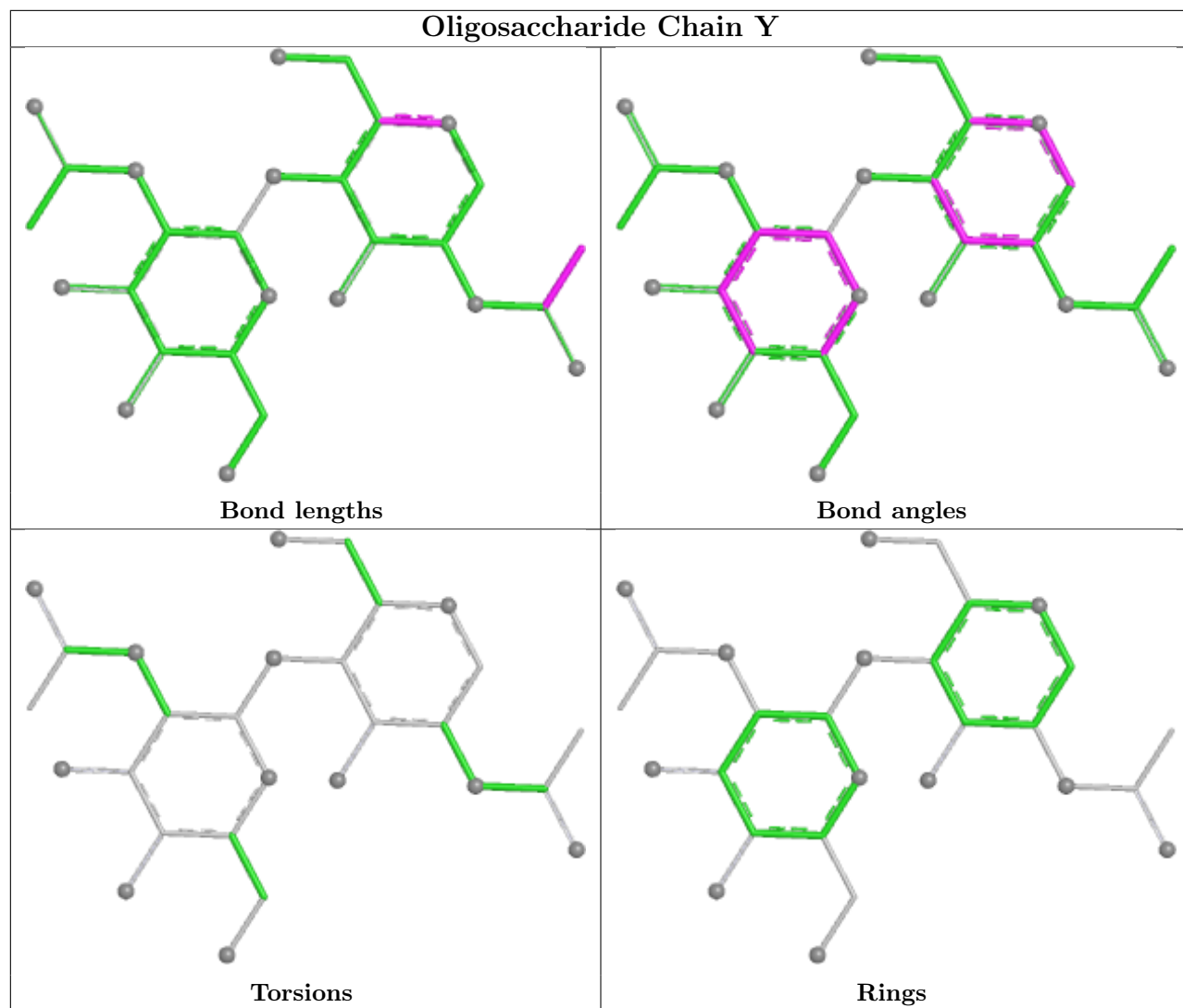


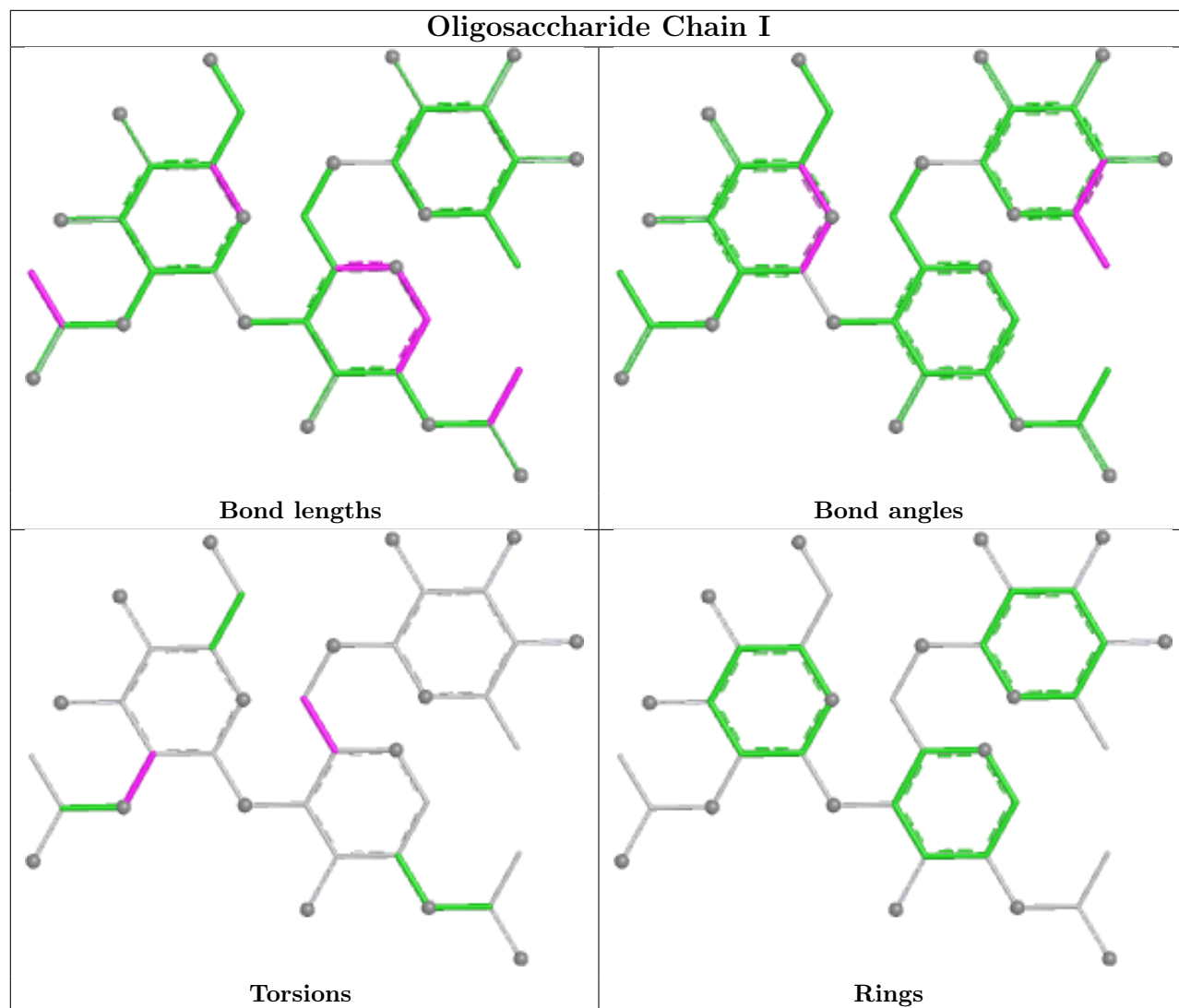


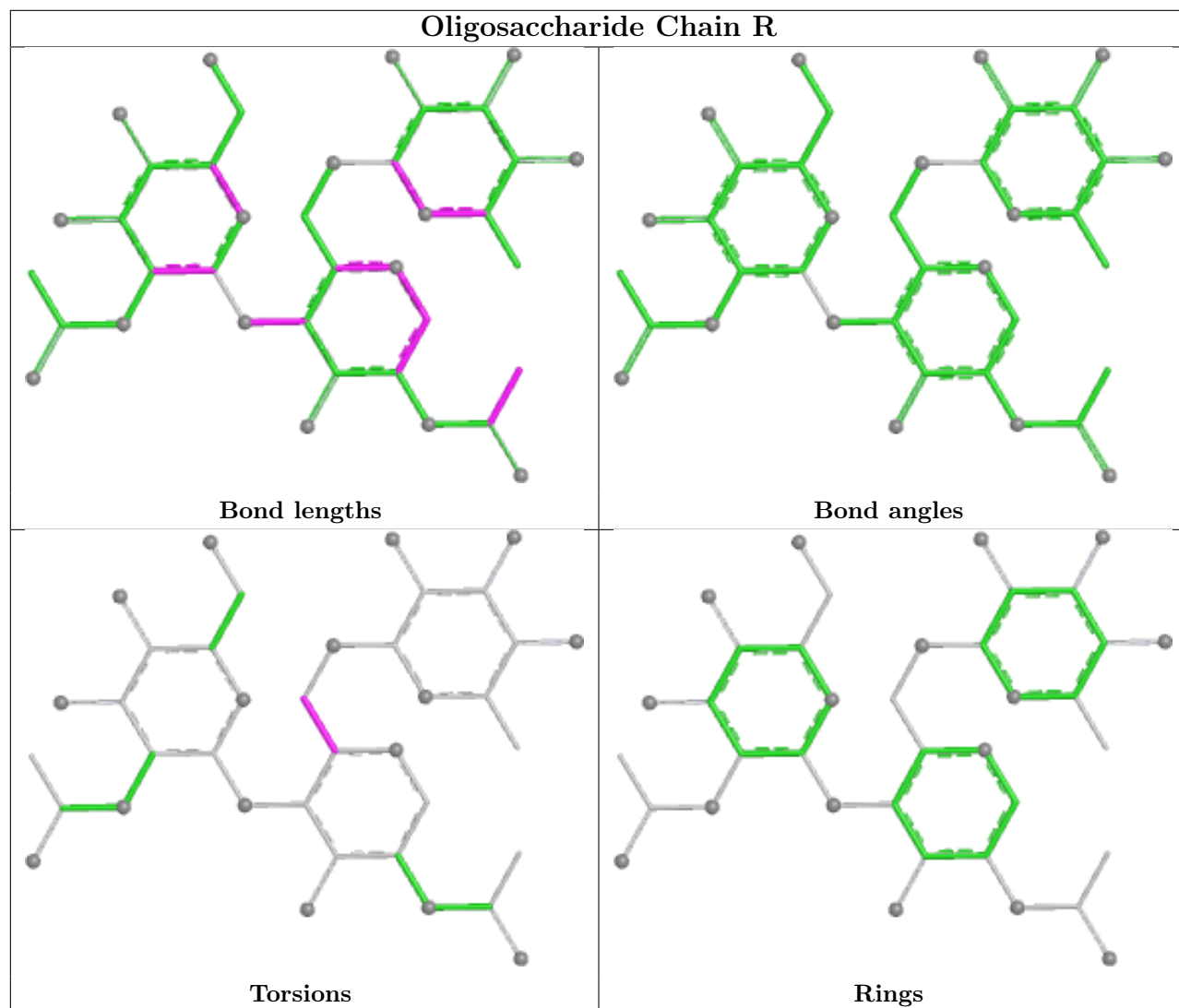


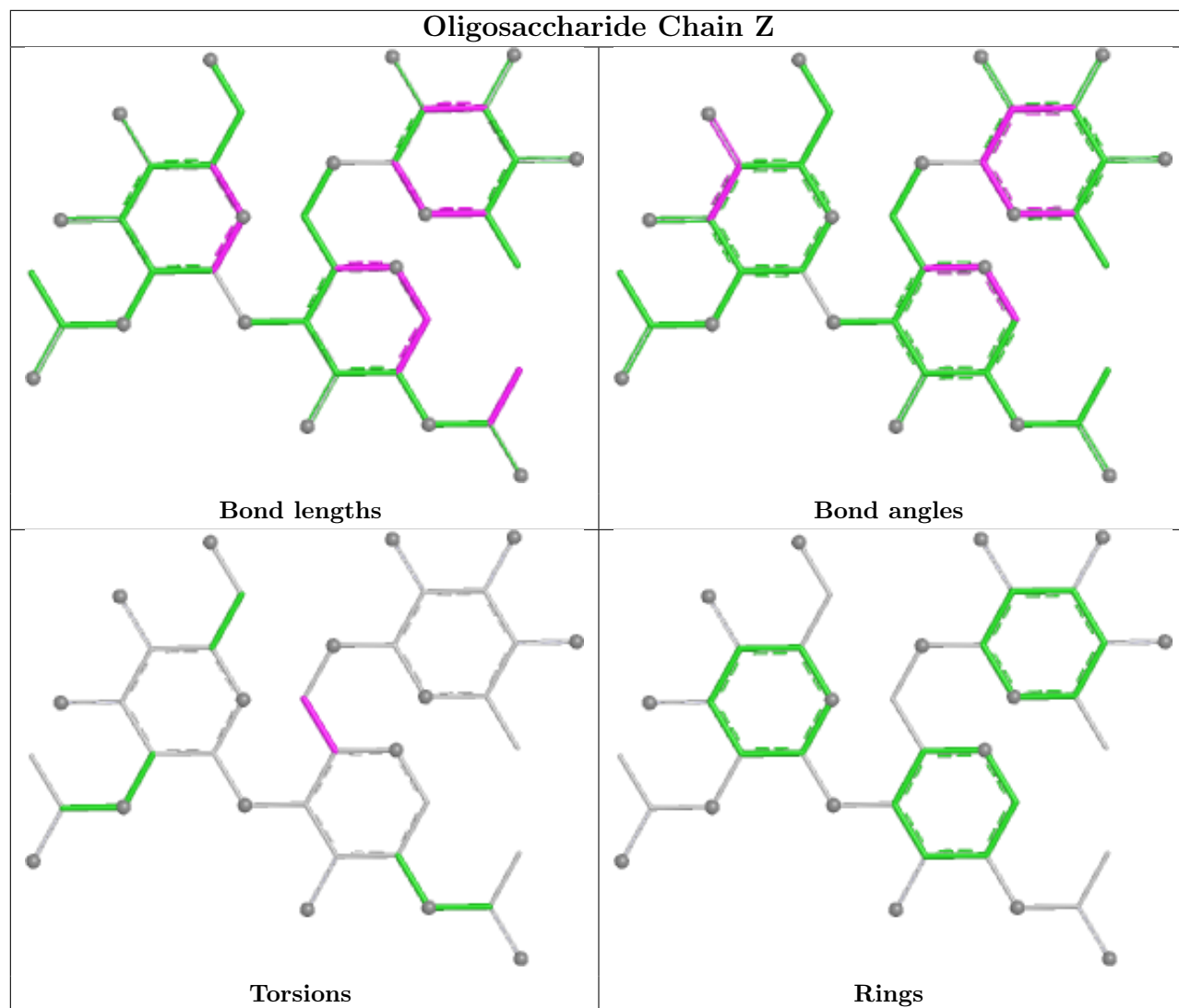


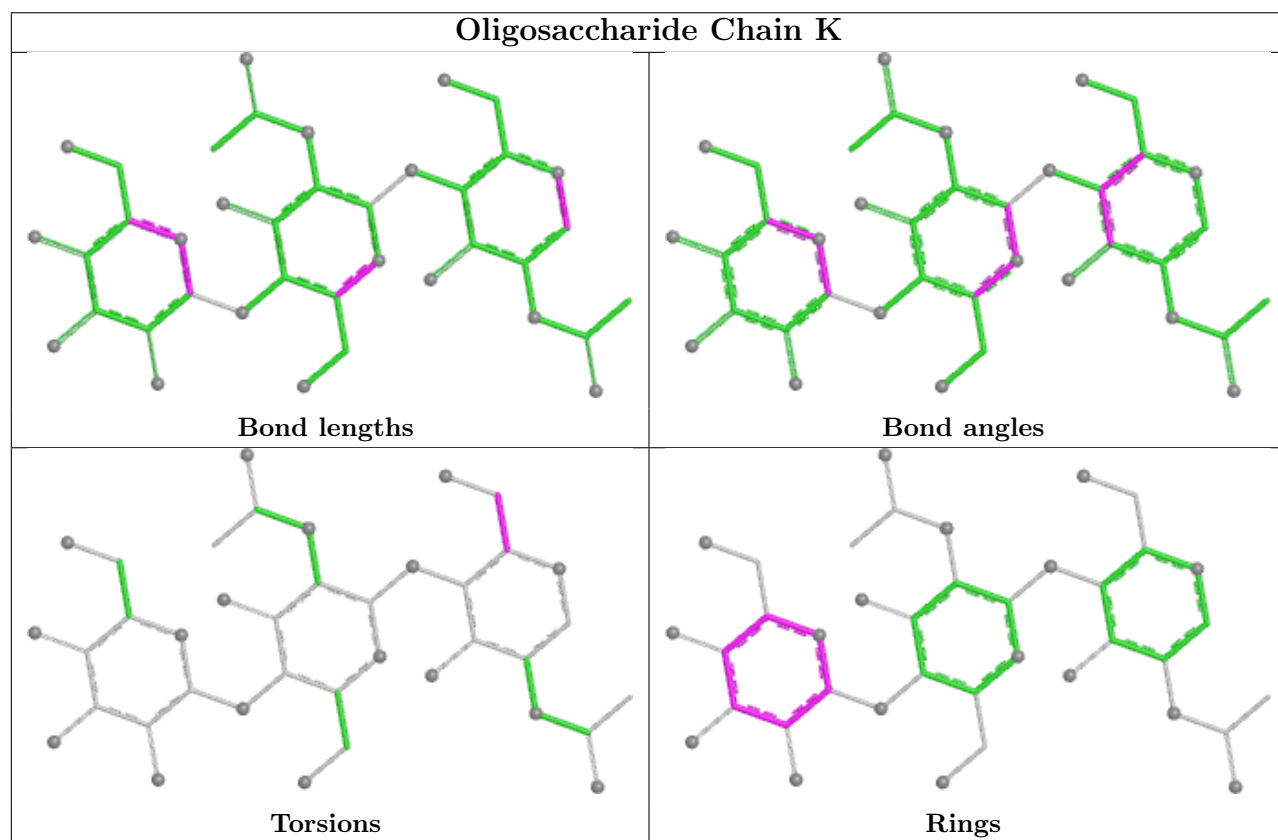
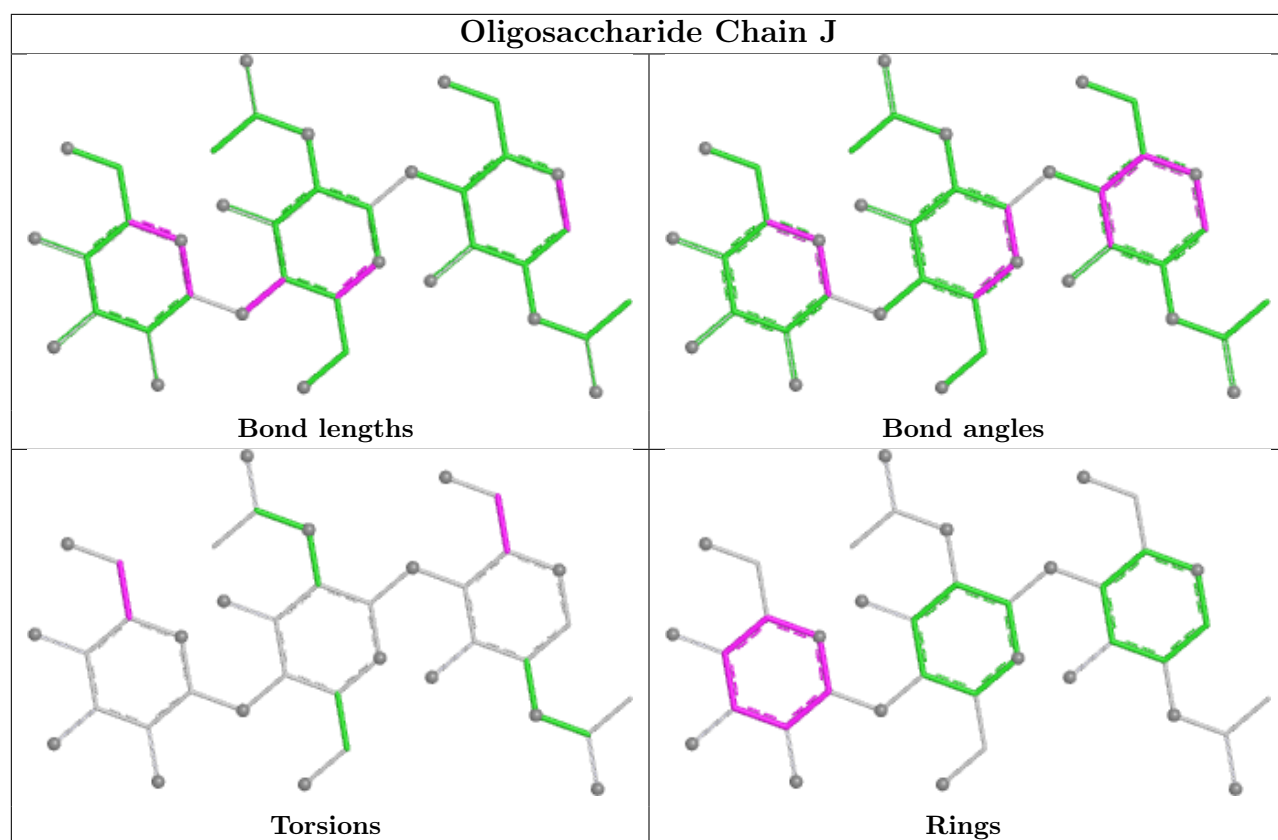


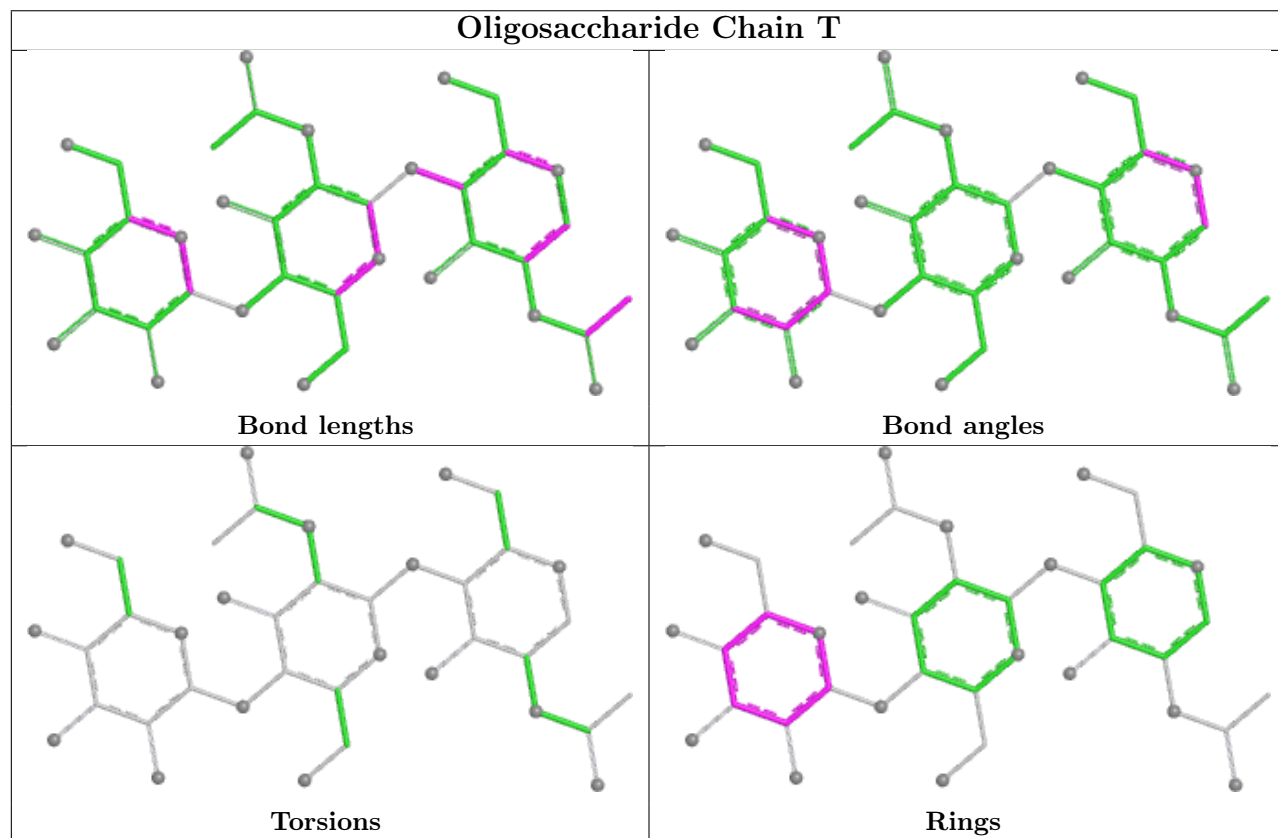
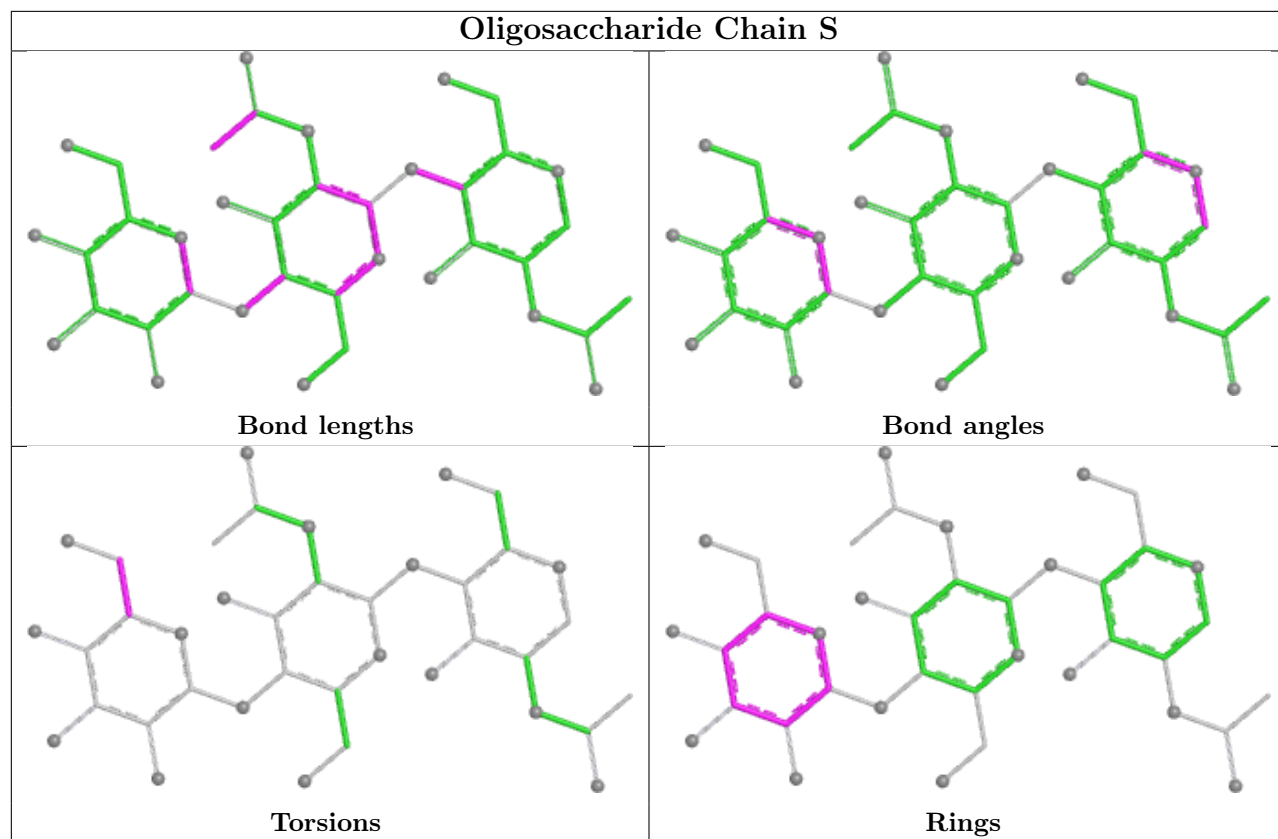


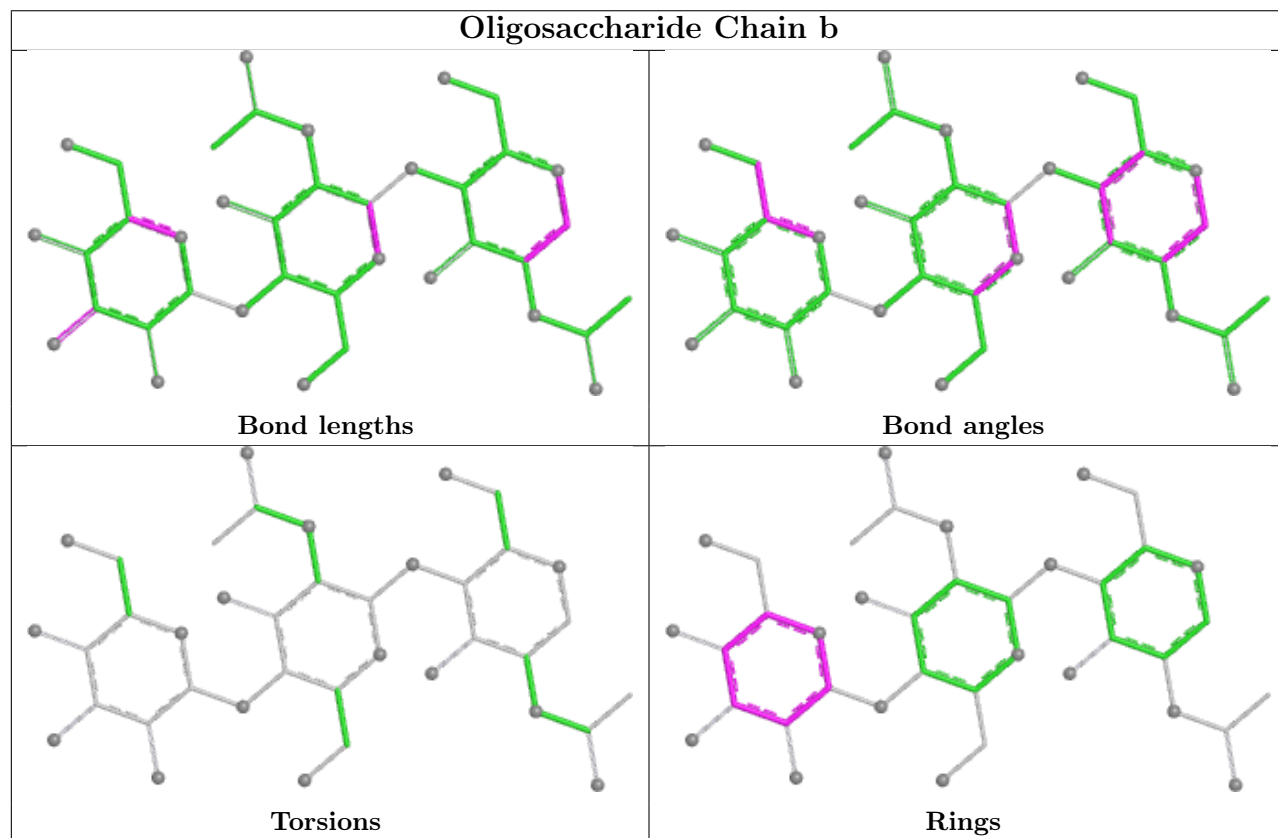
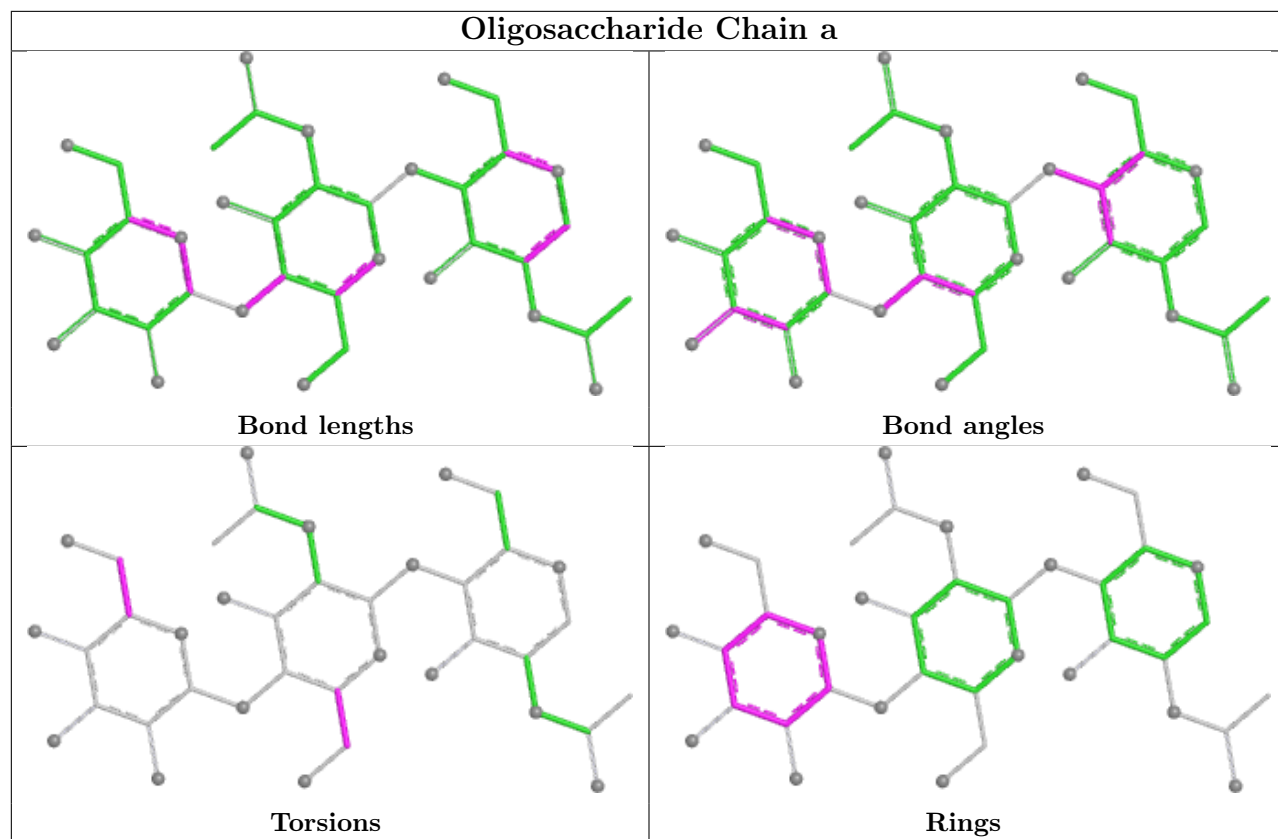












5.6 Ligand geometry

32 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	1403	1	14,14,15	0.28	0	17,19,21	0.51	0
5	NAG	A	1410	1	14,14,15	1.85	3 (21%)	17,19,21	1.02	1 (5%)
5	NAG	B	1401	1	14,14,15	1.26	2 (14%)	17,19,21	1.49	1 (5%)
5	NAG	B	1409	-	14,14,15	0.49	0	17,19,21	0.37	0
5	NAG	B	1406	-	14,14,15	0.19	0	17,19,21	0.63	0
5	NAG	C	1409	1	14,14,15	1.25	3 (21%)	17,19,21	0.72	0
5	NAG	B	1402	-	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	A	1409	1	14,14,15	1.45	2 (14%)	17,19,21	0.89	0
5	NAG	A	1405	-	14,14,15	0.33	0	17,19,21	0.61	0
5	NAG	A	1404	-	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	C	1406	1	14,14,15	1.40	2 (14%)	17,19,21	0.83	1 (5%)
5	NAG	C	1404	-	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	A	1406	1	14,14,15	1.24	2 (14%)	17,19,21	1.06	2 (11%)
5	NAG	A	1407	-	14,14,15	0.38	0	17,19,21	0.42	0
5	NAG	A	1402	-	14,14,15	0.27	0	17,19,21	0.50	0
5	NAG	B	1410	1	14,14,15	1.42	2 (14%)	17,19,21	0.76	0
5	NAG	C	1407	1	14,14,15	1.67	3 (21%)	17,19,21	1.36	3 (17%)
5	NAG	A	1411	1	14,14,15	1.35	3 (21%)	17,19,21	1.09	1 (5%)
5	NAG	A	1403	1	14,14,15	1.54	3 (21%)	17,19,21	1.72	2 (11%)
5	NAG	B	1408	1	14,14,15	1.27	2 (14%)	17,19,21	1.26	2 (11%)
5	NAG	C	1402	-	14,14,15	0.20	0	17,19,21	0.56	0
5	NAG	A	1408	-	14,14,15	0.19	0	17,19,21	0.46	0
5	NAG	C	1411	1	14,14,15	1.14	1 (7%)	17,19,21	1.16	2 (11%)
5	NAG	C	1410	-	14,14,15	0.29	0	17,19,21	0.44	0
5	NAG	C	1408	1	14,14,15	1.32	3 (21%)	17,19,21	1.09	1 (5%)
5	NAG	A	1401	-	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	B	1404	1	14,14,15	1.61	3 (21%)	17,19,21	1.00	1 (5%)
5	NAG	C	1405	-	14,14,15	0.21	0	17,19,21	0.56	0
5	NAG	B	1407	1	14,14,15	1.39	1 (7%)	17,19,21	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1403	1	14,14,15	0.28	0	17,19,21	0.42	0
5	NAG	C	1401	-	14,14,15	0.30	0	17,19,21	0.38	0
5	NAG	B	1405	1	14,14,15	1.19	1 (7%)	17,19,21	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1410	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1409	-	-	0/6/23/26	0/1/1/1
5	NAG	B	1406	-	-	2/6/23/26	0/1/1/1
5	NAG	C	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1402	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1405	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1404	-	-	2/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1404	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1407	-	-	4/6/23/26	0/1/1/1
5	NAG	A	1402	-	-	2/6/23/26	0/1/1/1
5	NAG	B	1410	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1411	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1402	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1408	-	-	2/6/23/26	0/1/1/1
5	NAG	C	1411	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1410	-	-	1/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1401	-	-	2/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1405	-	-	0/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1401	-	-	2/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	0/6/23/26	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1410	NAG	O5-C5	4.31	1.51	1.43
5	A	1410	NAG	C1-C2	4.17	1.58	1.52
5	B	1410	NAG	O5-C5	3.69	1.50	1.43
5	B	1407	NAG	O5-C5	3.58	1.50	1.43
5	C	1407	NAG	C1-C2	3.46	1.57	1.52
5	B	1404	NAG	O5-C5	3.32	1.49	1.43
5	A	1409	NAG	O5-C5	3.29	1.49	1.43
5	C	1407	NAG	O5-C5	3.27	1.49	1.43
5	B	1404	NAG	O5-C1	3.01	1.48	1.43
5	B	1404	NAG	C1-C2	3.00	1.56	1.52
5	A	1403	NAG	C1-C2	2.98	1.56	1.52
5	A	1403	NAG	O5-C5	2.93	1.49	1.43
5	B	1405	NAG	O5-C5	2.77	1.48	1.43
5	A	1406	NAG	C1-C2	2.77	1.56	1.52
5	C	1411	NAG	O5-C5	2.73	1.48	1.43
5	C	1408	NAG	C1-C2	2.69	1.56	1.52
5	B	1408	NAG	C1-C2	2.68	1.56	1.52
5	A	1411	NAG	C1-C2	2.62	1.55	1.52
5	B	1408	NAG	O5-C5	2.54	1.48	1.43
5	A	1411	NAG	O5-C1	2.52	1.47	1.43
5	A	1411	NAG	O5-C5	2.48	1.48	1.43
5	B	1401	NAG	C1-C2	2.47	1.55	1.52
5	B	1401	NAG	O5-C5	2.46	1.48	1.43
5	C	1408	NAG	O5-C5	2.42	1.48	1.43
5	A	1406	NAG	O5-C5	2.42	1.48	1.43
5	A	1409	NAG	C1-C2	2.29	1.55	1.52
5	C	1406	NAG	C8-C7	2.29	1.55	1.50
5	A	1403	NAG	C3-C2	2.29	1.57	1.52
5	C	1409	NAG	C8-C7	2.22	1.55	1.50
5	C	1406	NAG	C3-C2	2.16	1.57	1.52
5	C	1409	NAG	O5-C5	2.15	1.47	1.43
5	B	1410	NAG	C8-C7	2.15	1.55	1.50
5	C	1409	NAG	C1-C2	2.11	1.55	1.52
5	C	1407	NAG	O5-C1	2.11	1.47	1.43
5	A	1410	NAG	C8-C7	2.10	1.54	1.50
5	C	1408	NAG	O5-C1	2.06	1.47	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1403	NAG	C1-O5-C5	5.51	119.57	112.19
5	B	1401	NAG	C1-O5-C5	4.78	118.59	112.19
5	A	1411	NAG	C2-N2-C7	3.46	127.54	122.90
5	B	1408	NAG	C3-C4-C5	3.42	116.43	110.23
5	C	1408	NAG	C1-O5-C5	2.97	116.17	112.19
5	C	1411	NAG	C1-O5-C5	2.93	116.12	112.19
5	A	1410	NAG	C1-O5-C5	2.86	116.02	112.19
5	C	1407	NAG	O5-C1-C2	-2.73	107.07	111.29
5	C	1407	NAG	C3-C4-C5	2.61	114.97	110.23
5	A	1403	NAG	C2-N2-C7	2.59	126.37	122.90
5	C	1407	NAG	C1-C2-N2	2.55	114.45	110.43
5	C	1406	NAG	C4-C3-C2	-2.55	107.28	111.02
5	B	1408	NAG	C4-C3-C2	-2.47	107.41	111.02
5	B	1404	NAG	C4-C3-C2	2.46	114.62	111.02
5	C	1411	NAG	C3-C4-C5	2.25	114.32	110.23
5	A	1406	NAG	O5-C5-C6	2.08	111.72	107.66
5	A	1406	NAG	O5-C5-C4	-2.02	105.92	110.83

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1404	NAG	C4-C5-C6-O6
5	A	1408	NAG	O5-C5-C6-O6
5	B	1406	NAG	O5-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	A	1404	NAG	O5-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	A	1405	NAG	O5-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	A	1408	NAG	C4-C5-C6-O6
5	B	1406	NAG	C4-C5-C6-O6
5	A	1402	NAG	O5-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	A	1405	NAG	C4-C5-C6-O6
5	C	1401	NAG	C4-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	A	1407	NAG	C4-C5-C6-O6
5	C	1402	NAG	C4-C5-C6-O6
5	C	1401	NAG	O5-C5-C6-O6
5	A	1402	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1407	NAG	O5-C5-C6-O6
5	A	1407	NAG	C3-C2-N2-C7
5	B	1404	NAG	C8-C7-N2-C2
5	C	1410	NAG	O5-C5-C6-O6
5	A	1407	NAG	C1-C2-N2-C7

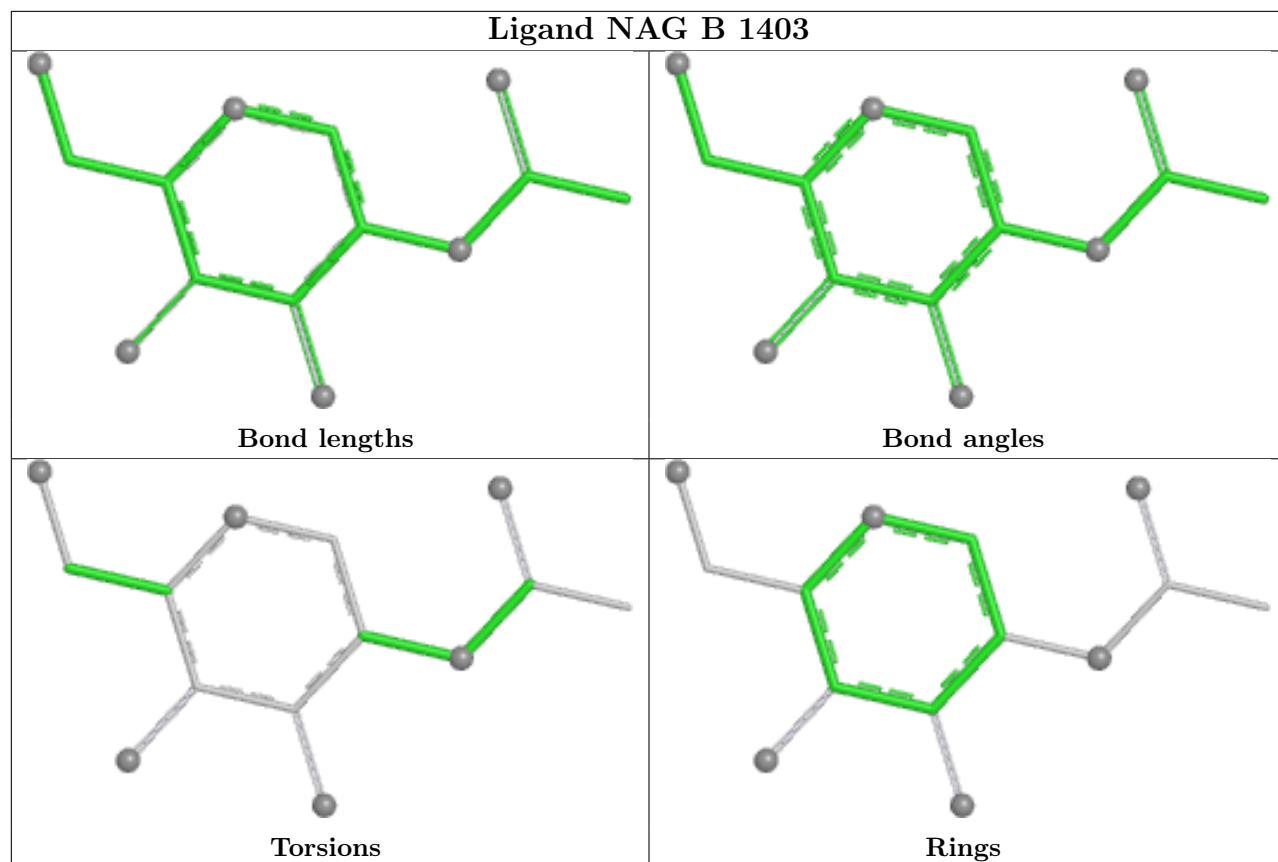
There are no ring outliers.

14 monomers are involved in 50 short contacts:

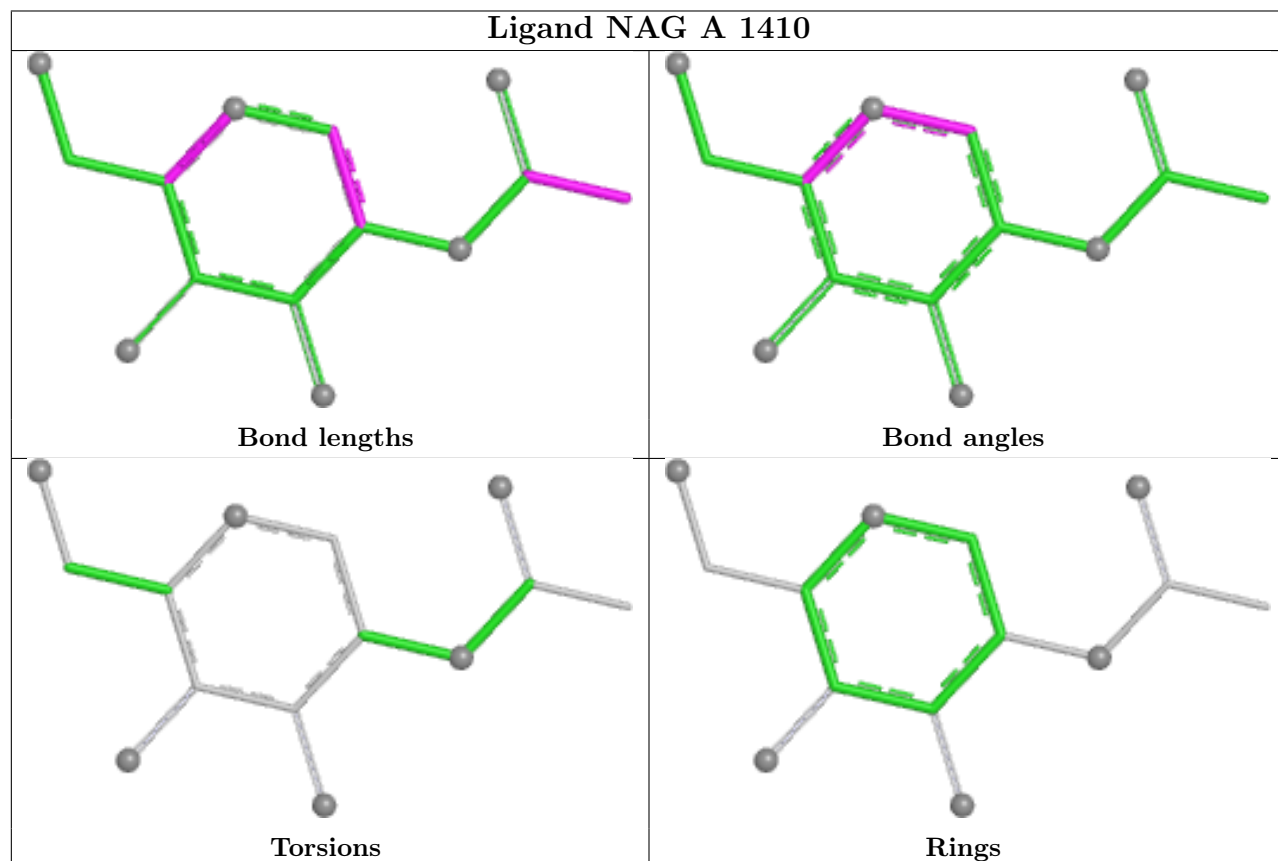
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1409	NAG	4	0
5	B	1406	NAG	6	0
5	B	1402	NAG	2	0
5	A	1405	NAG	5	0
5	A	1404	NAG	2	0
5	C	1404	NAG	3	0
5	A	1407	NAG	5	0
5	A	1402	NAG	5	0
5	C	1402	NAG	2	0
5	A	1408	NAG	6	0
5	C	1410	NAG	4	0
5	A	1401	NAG	3	0
5	C	1405	NAG	2	0
5	C	1403	NAG	1	0

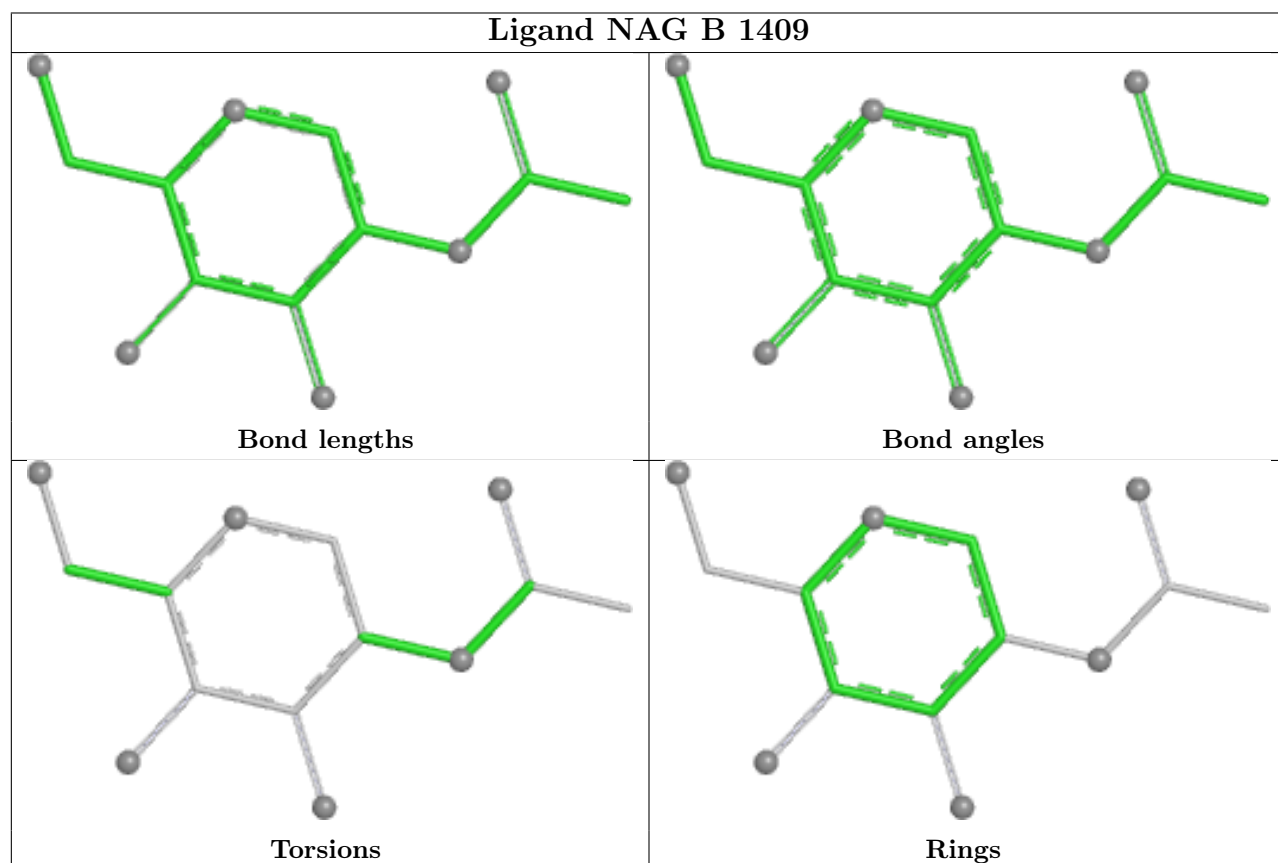
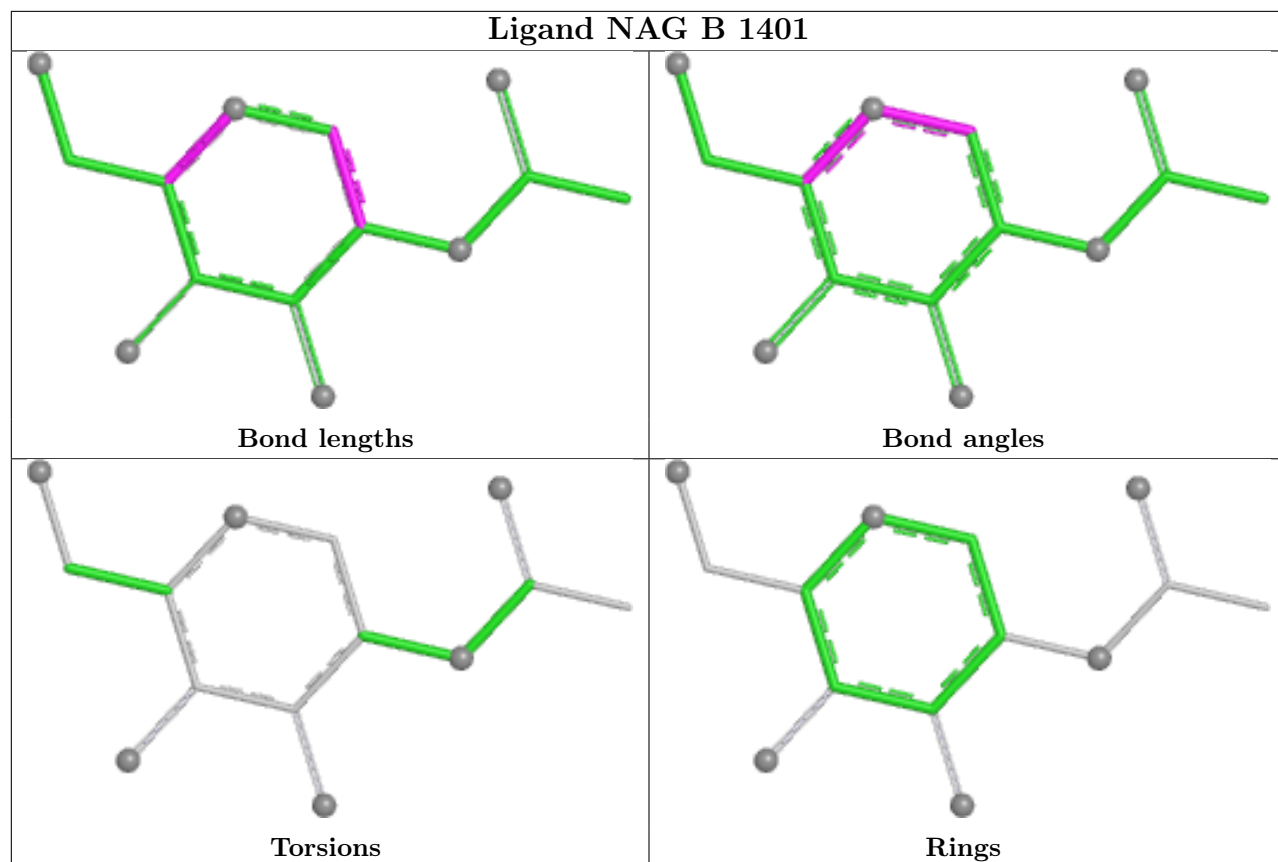
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand NAG B 1403

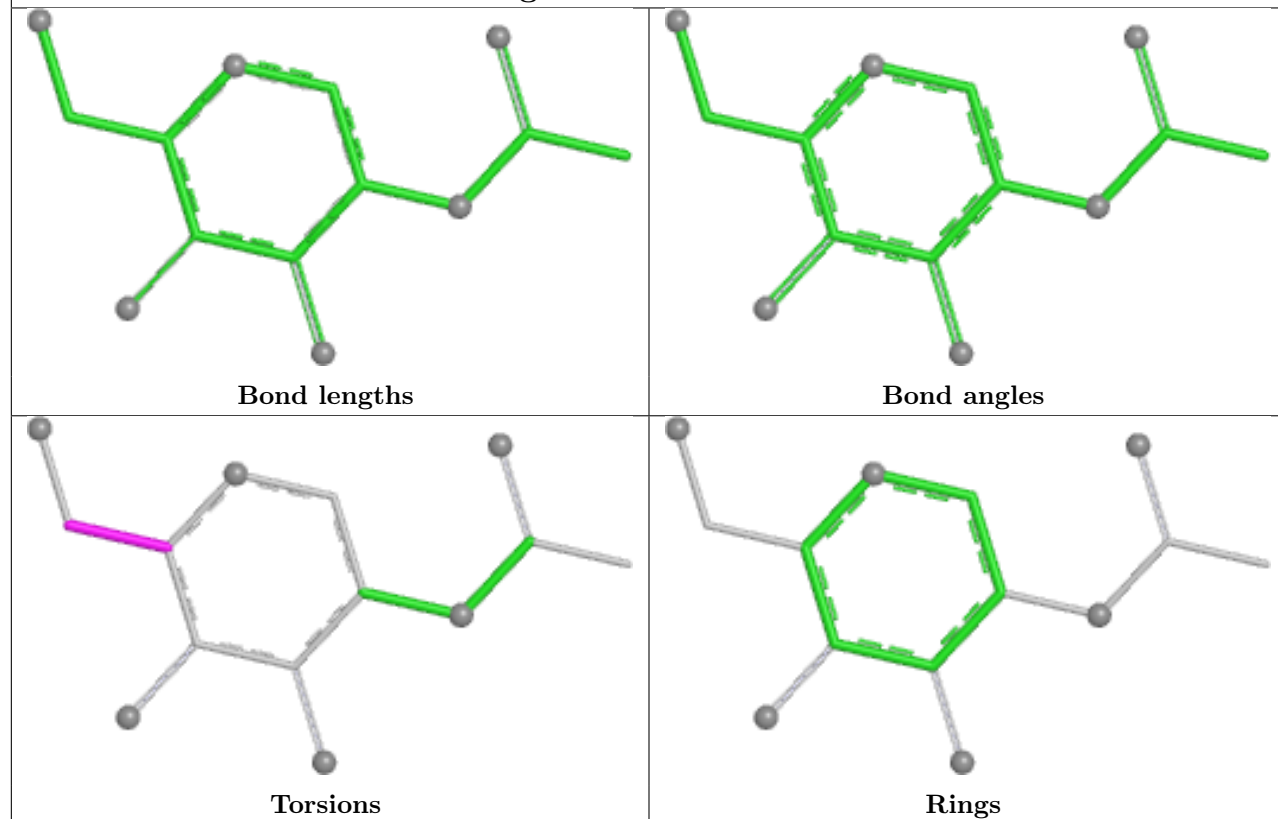


Ligand NAG A 1410

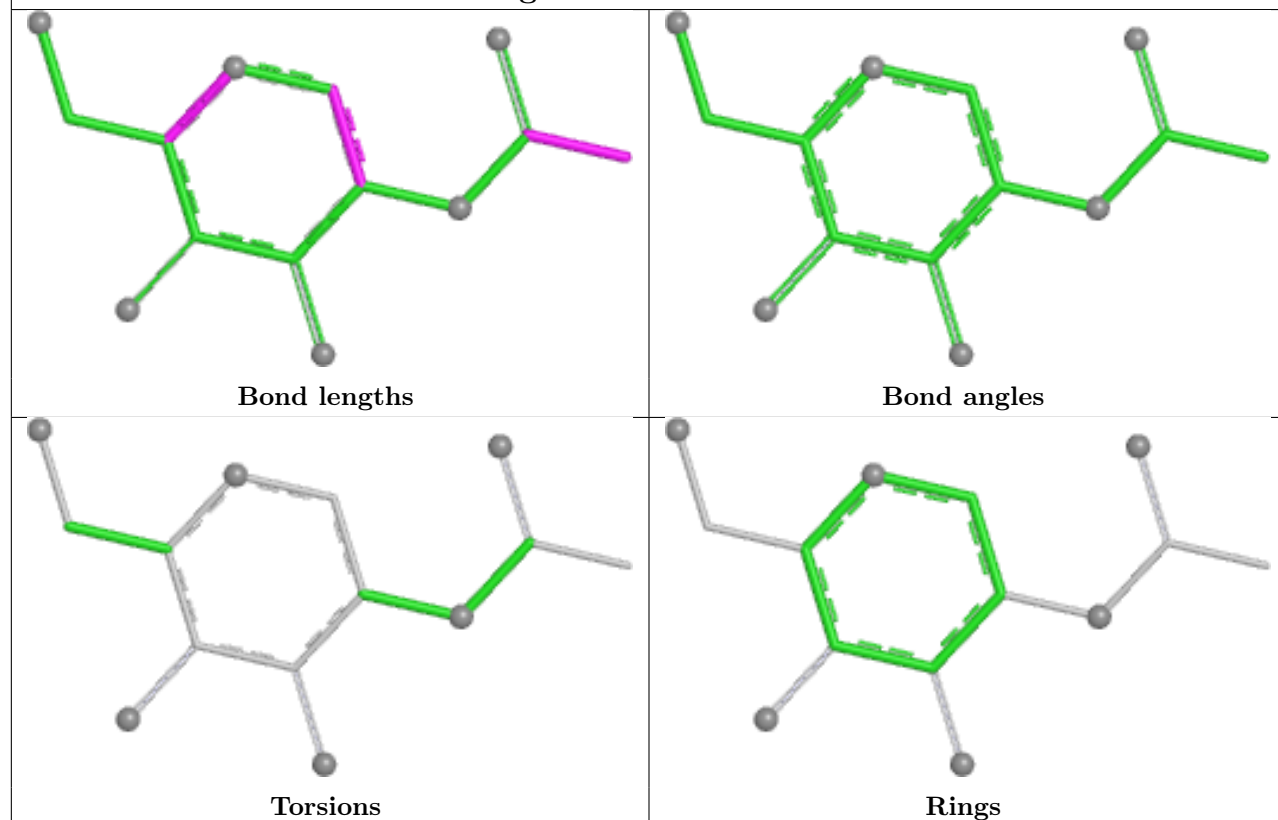


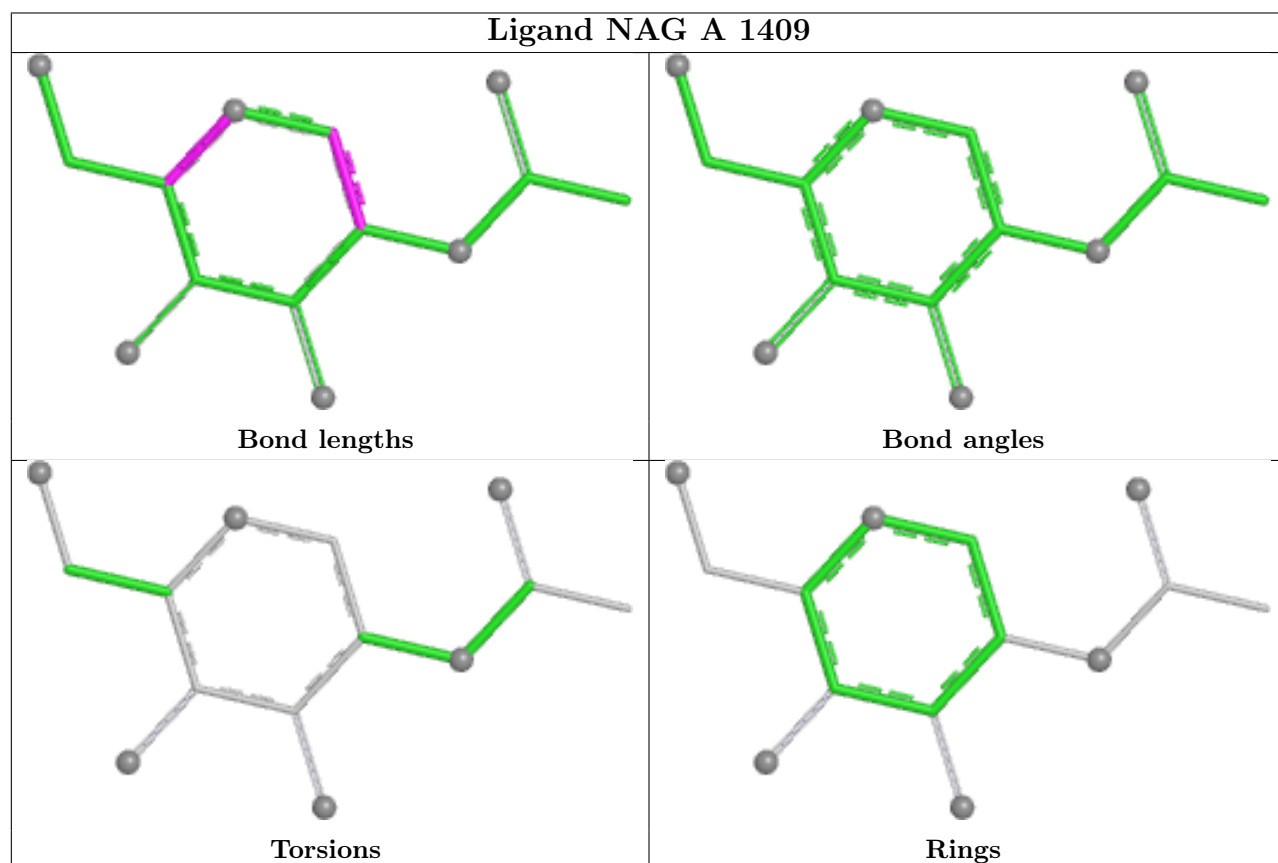
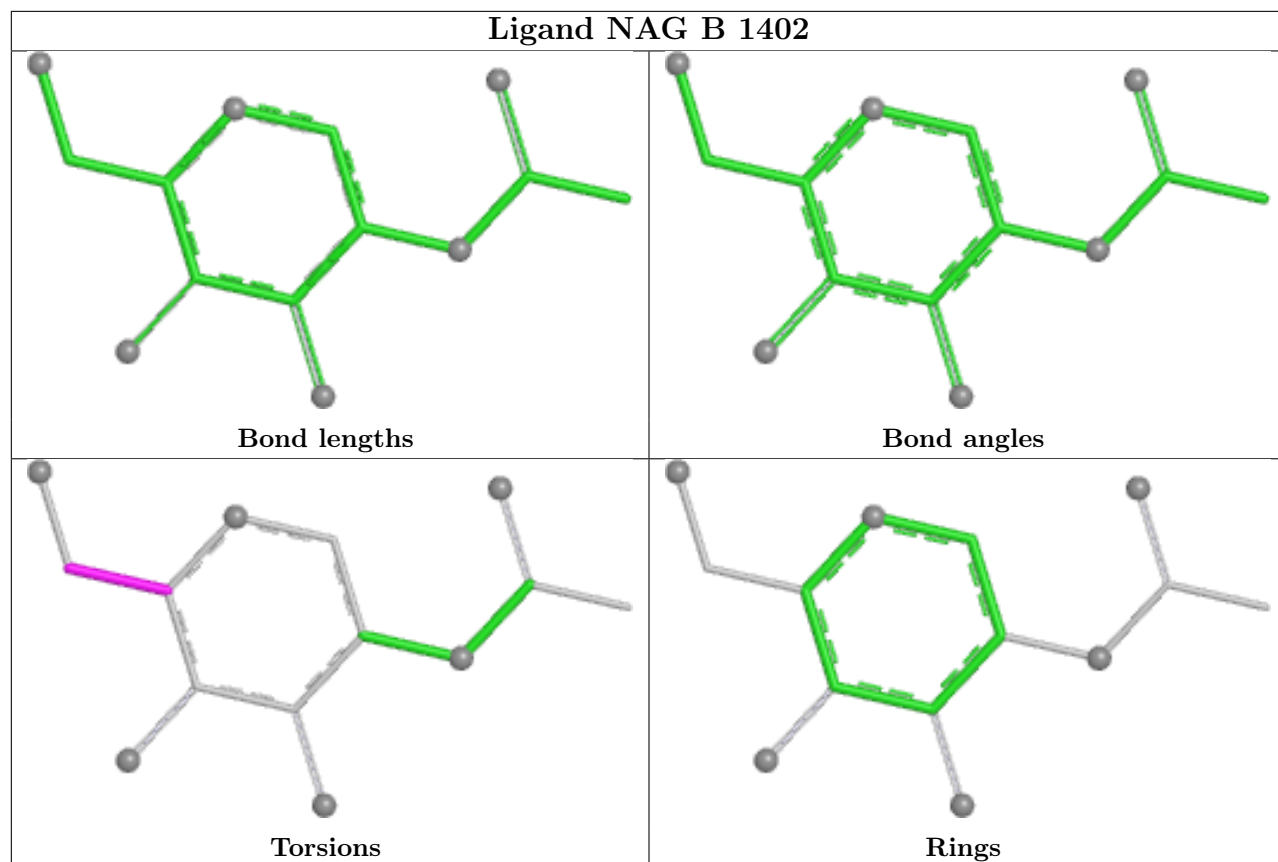


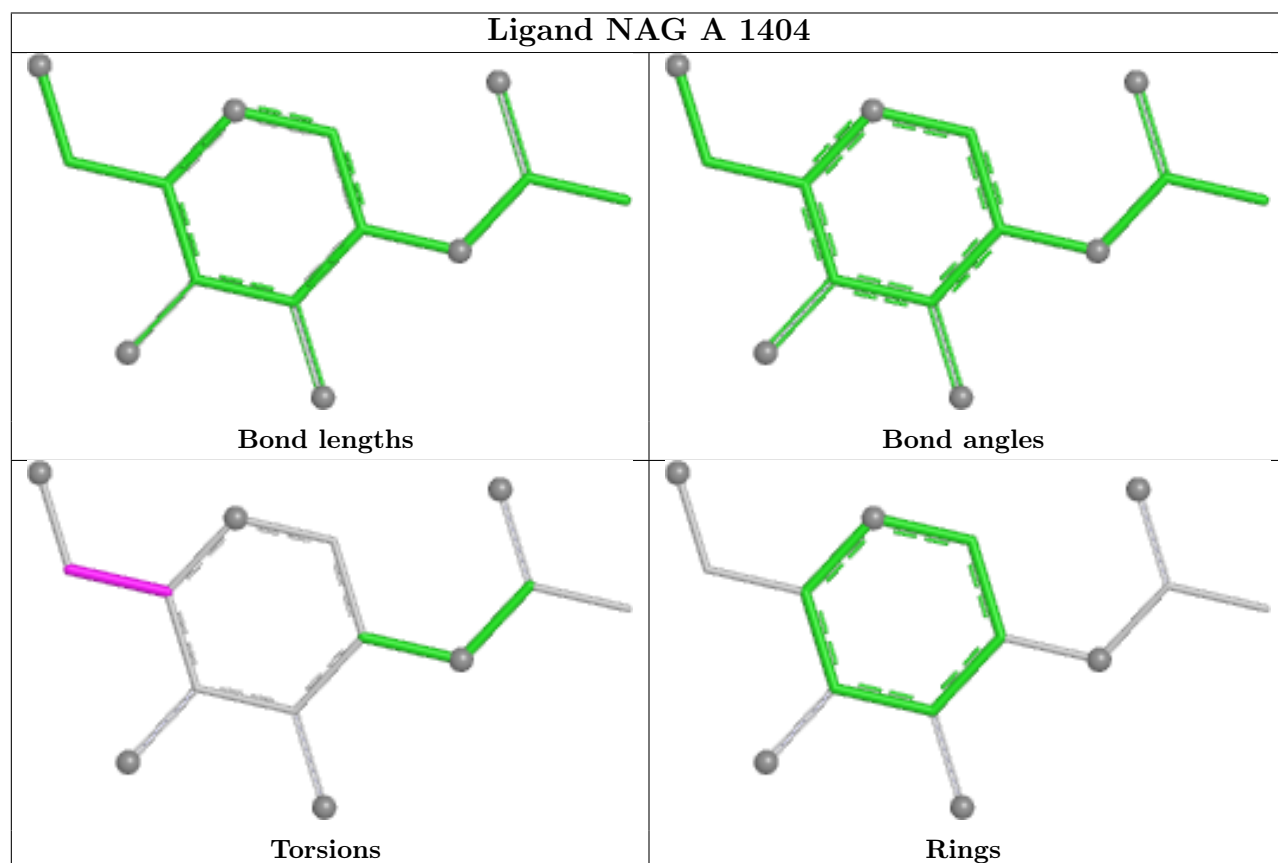
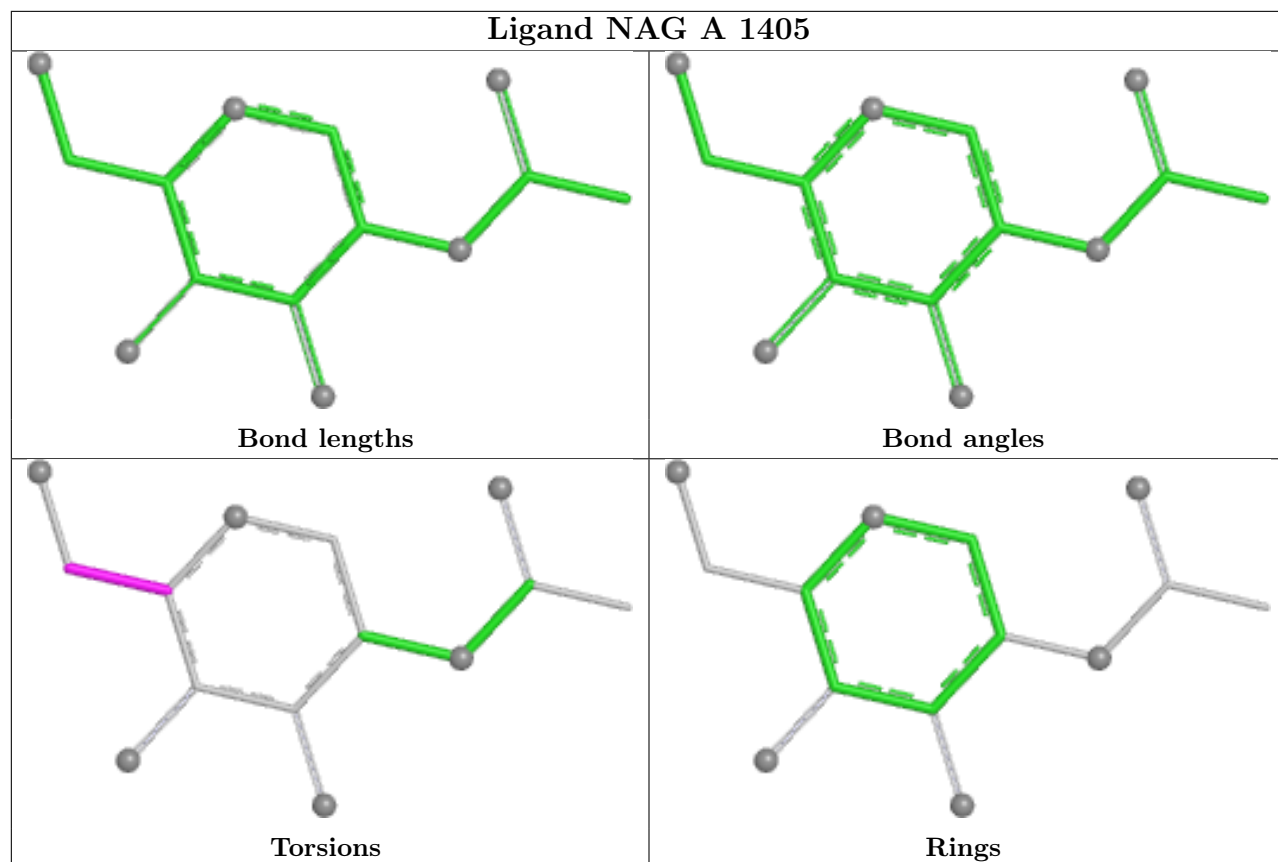
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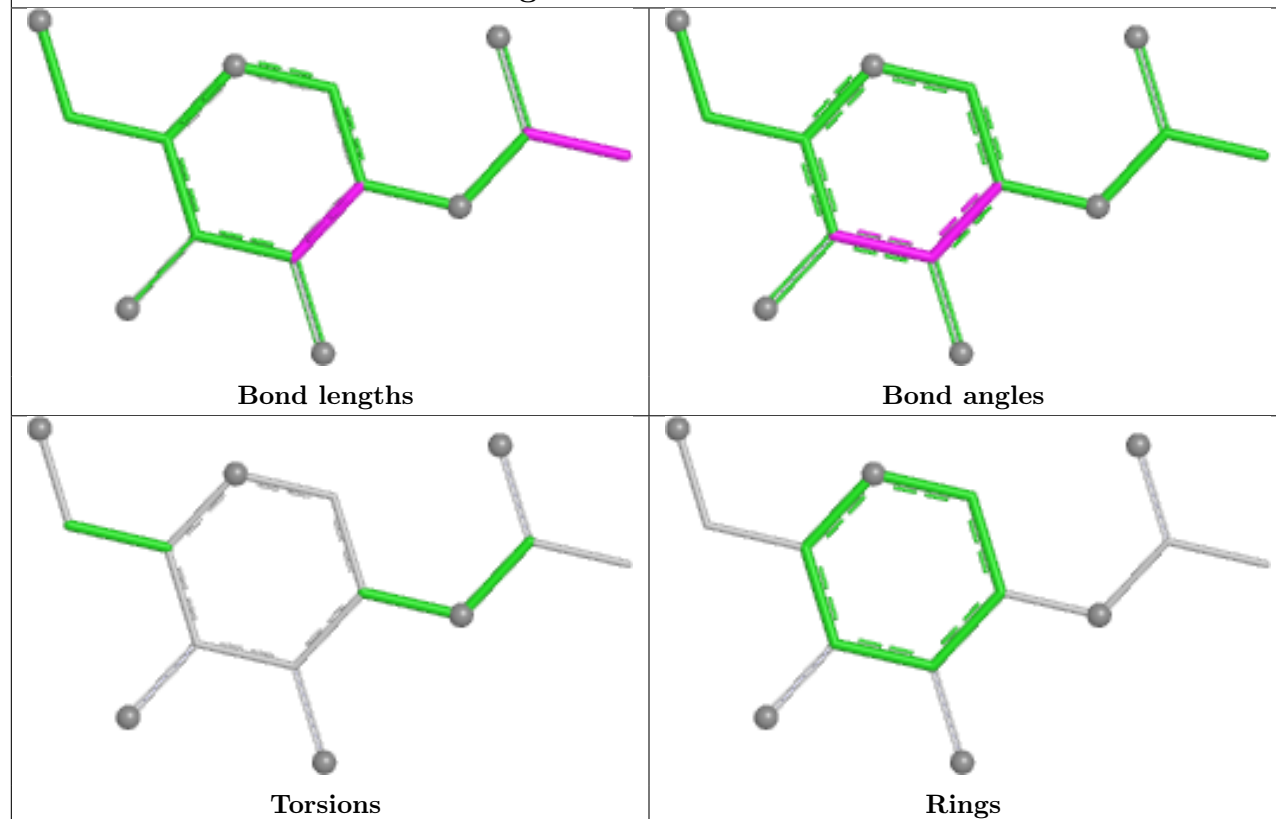
Ligand NAG C 1409



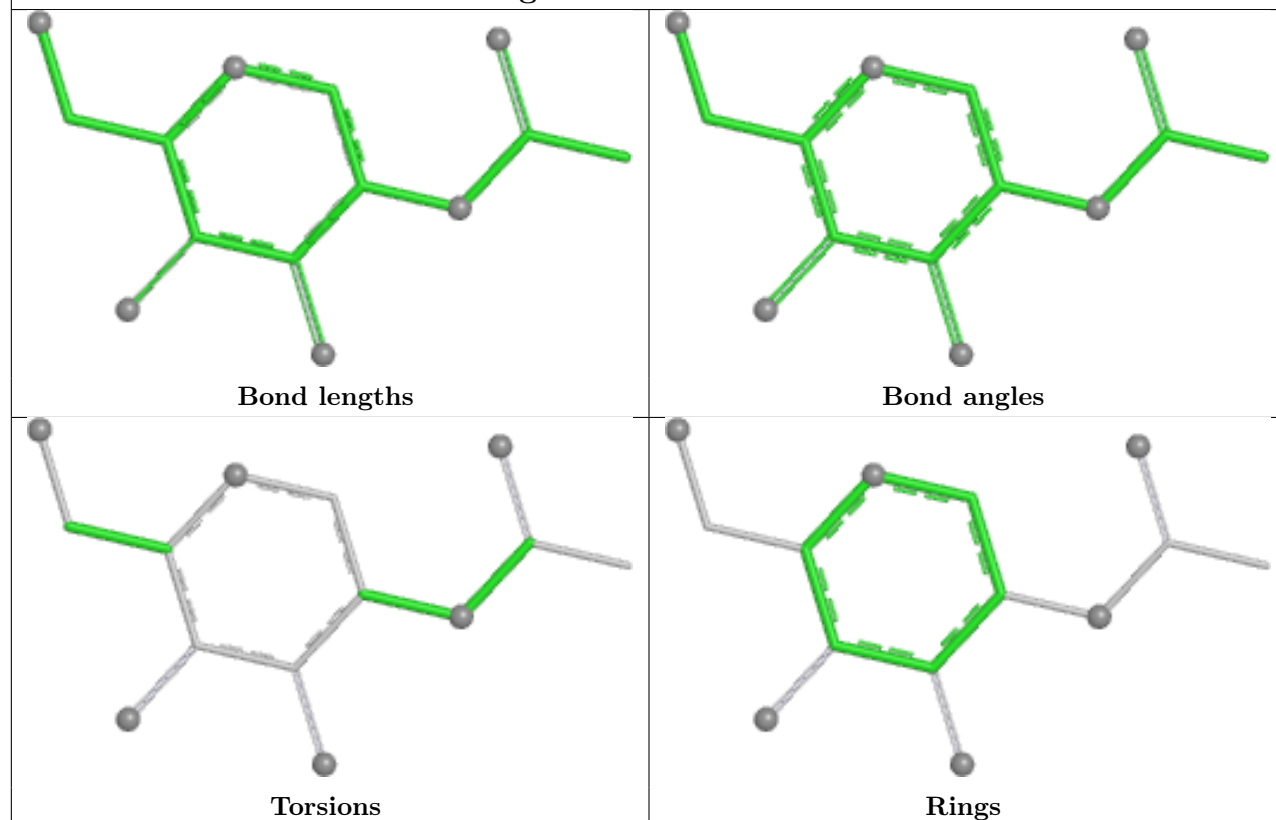


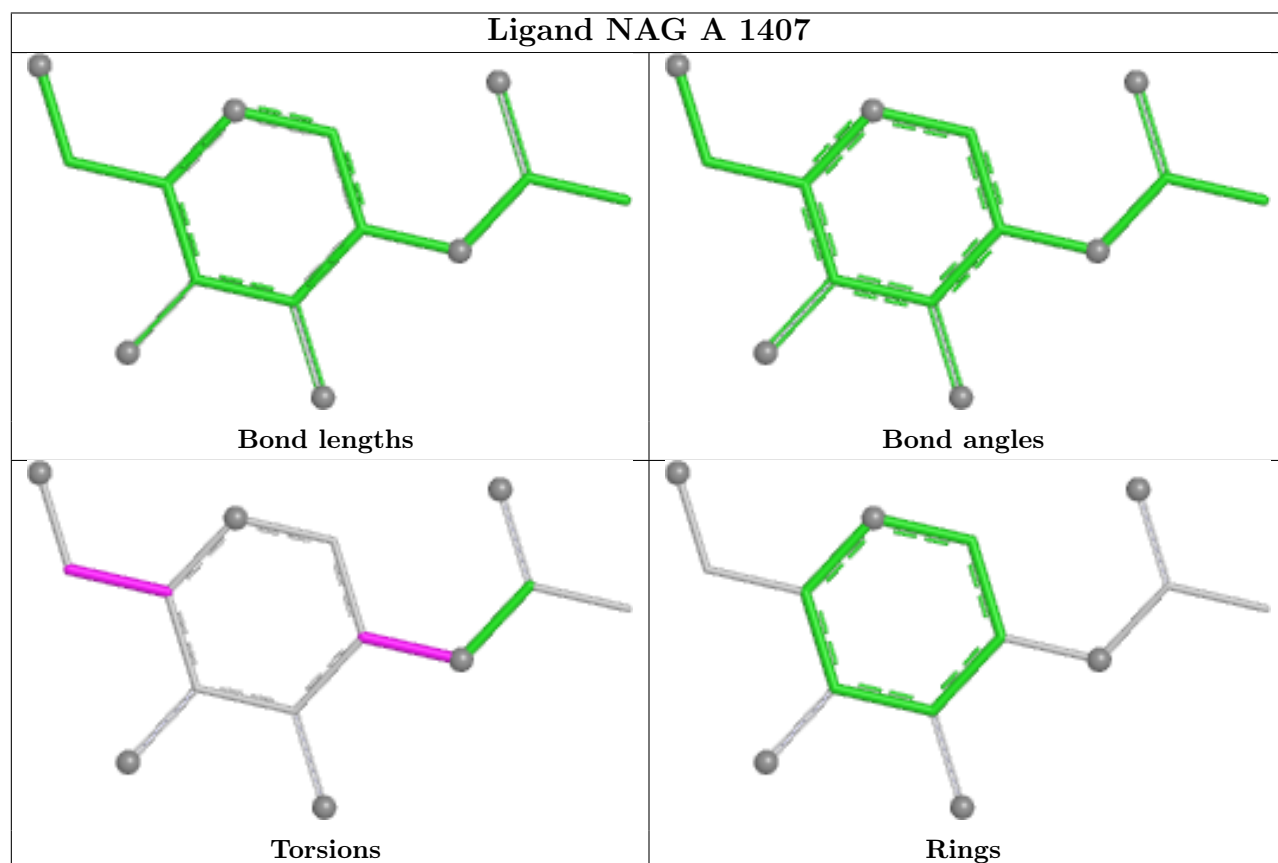
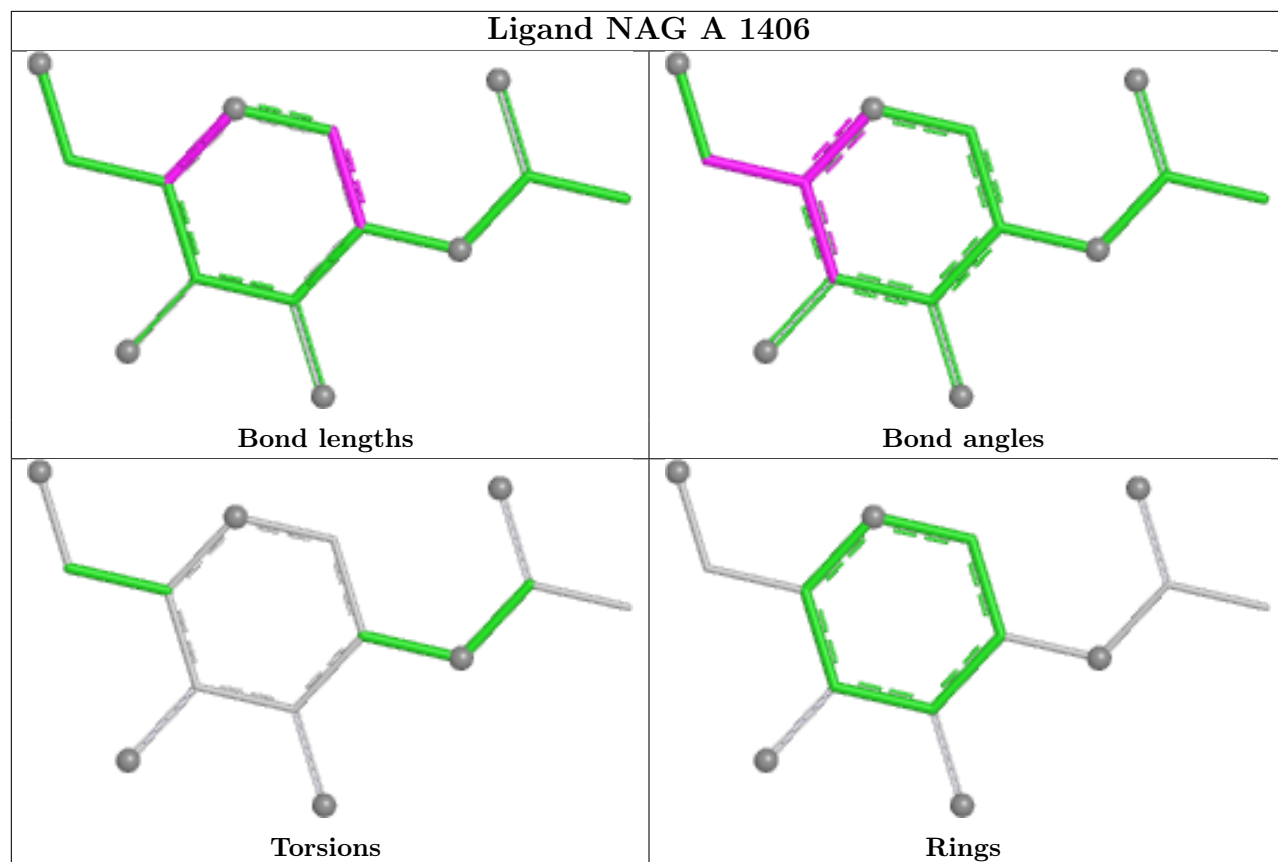


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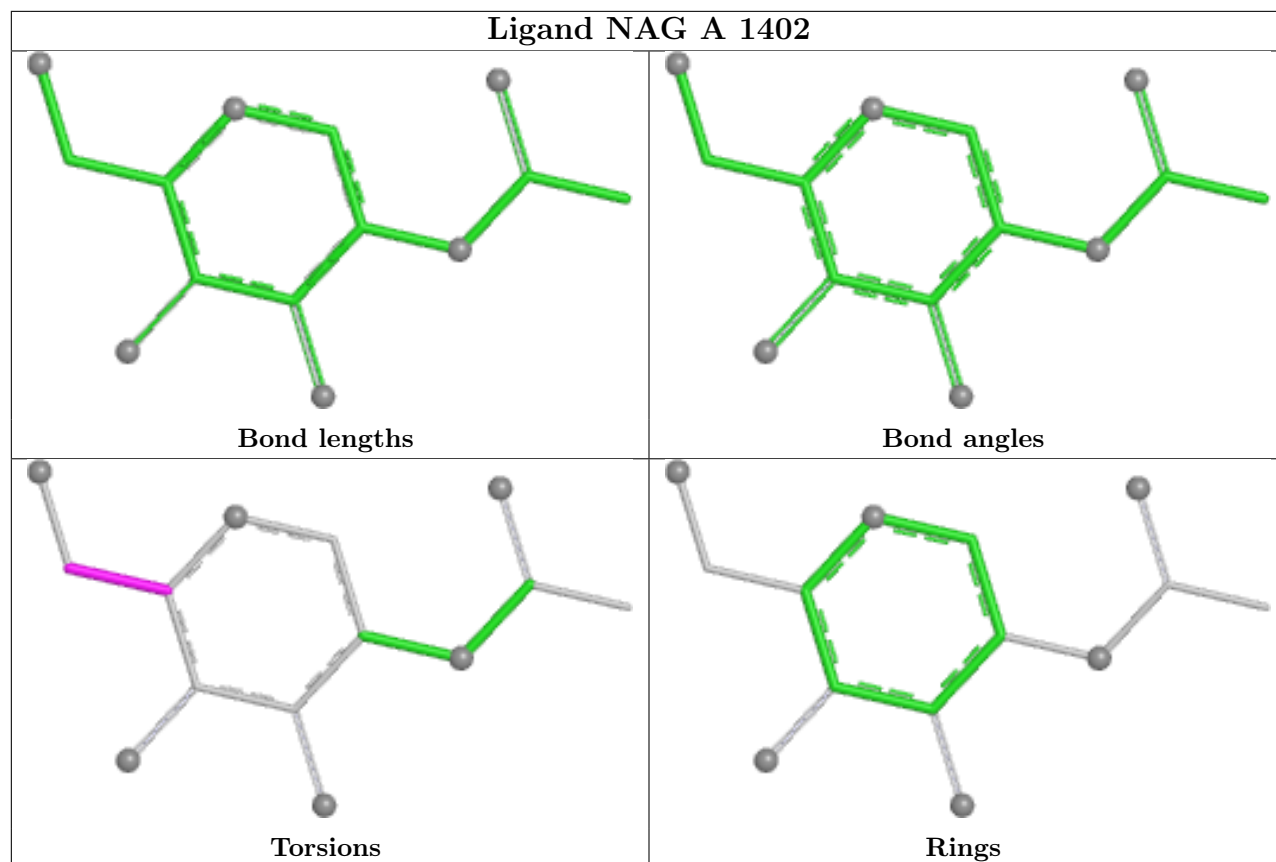


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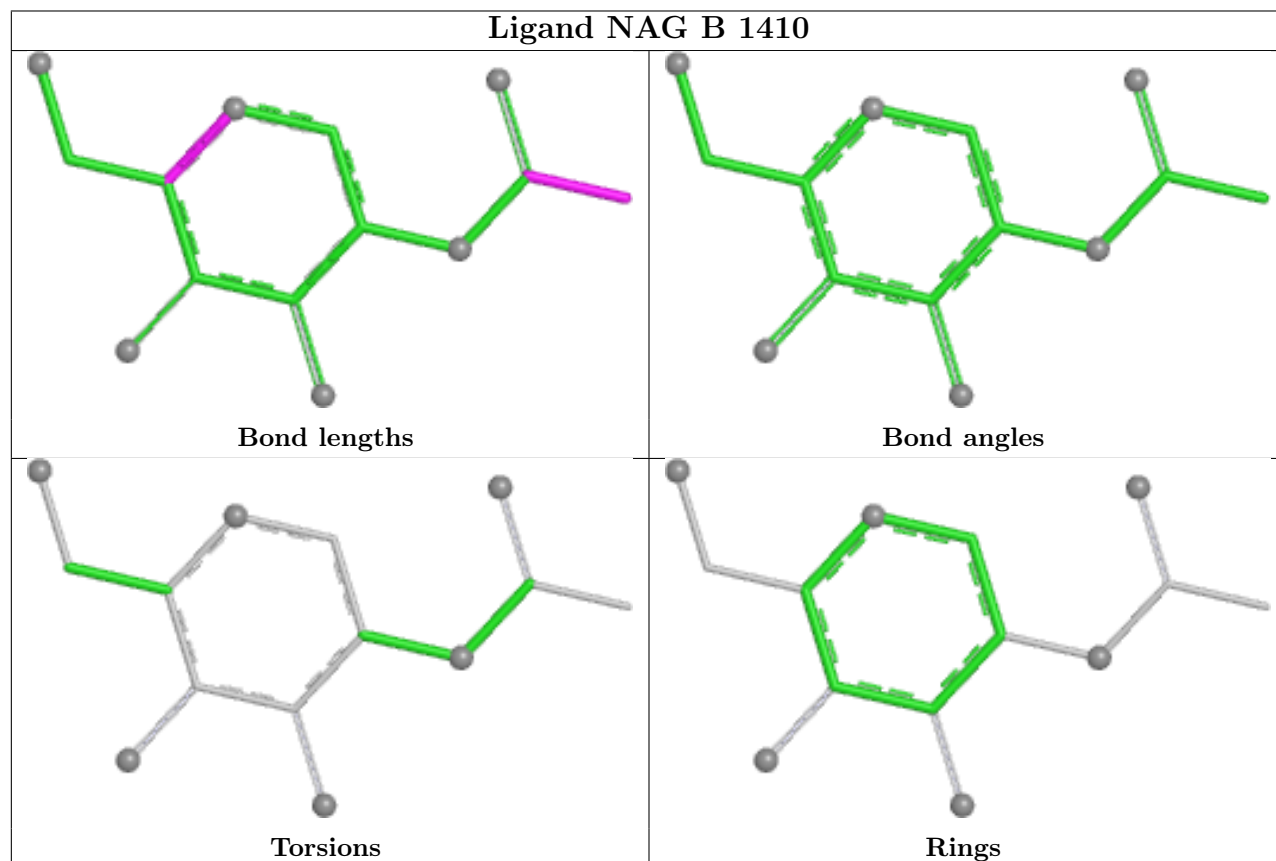




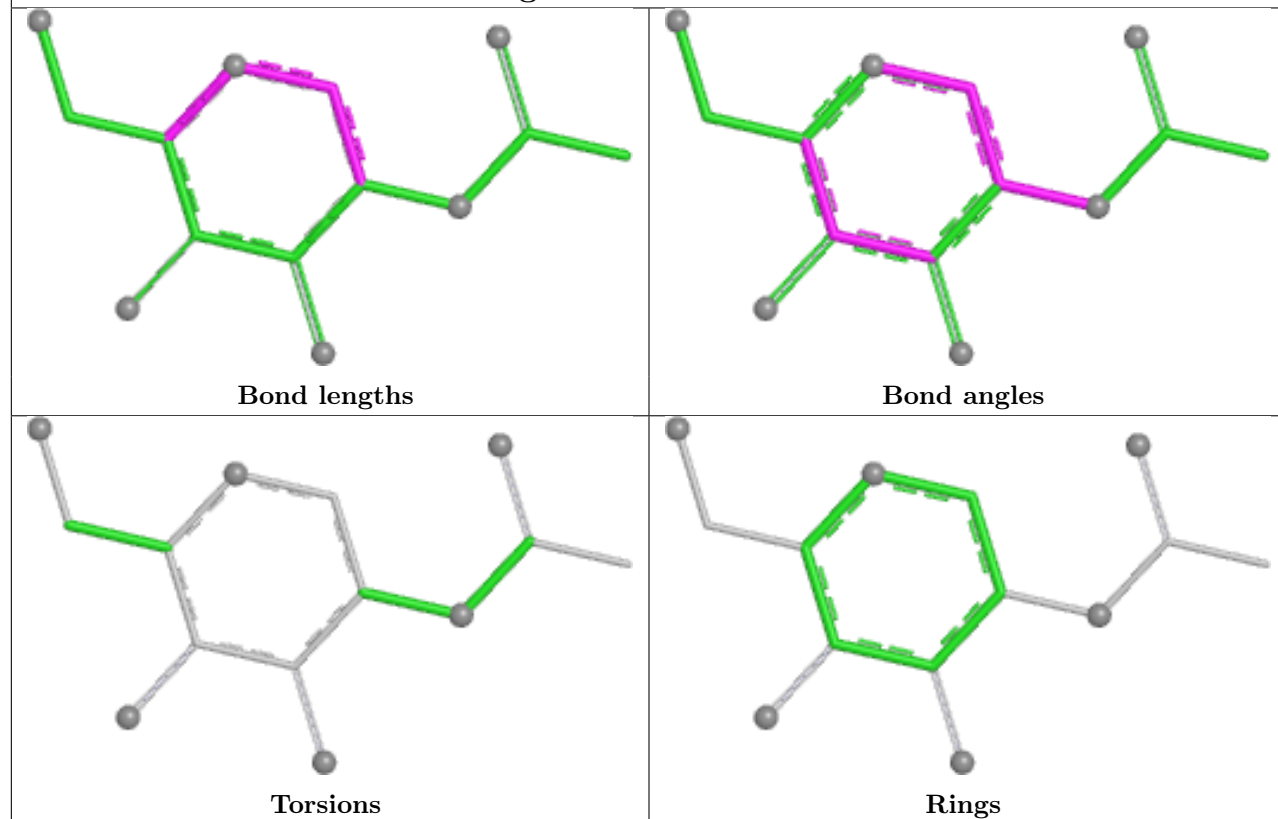
Ligand NAG A 1402



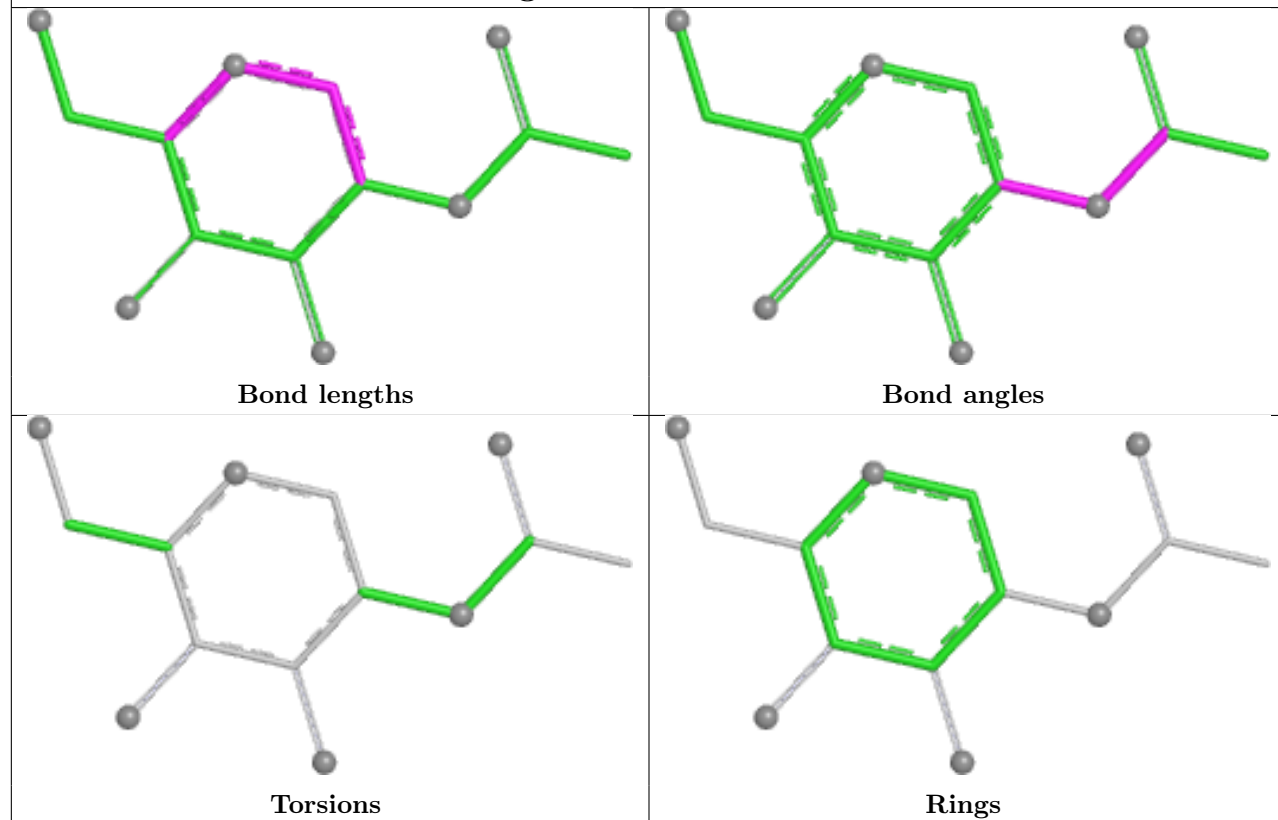
Ligand NAG B 1410



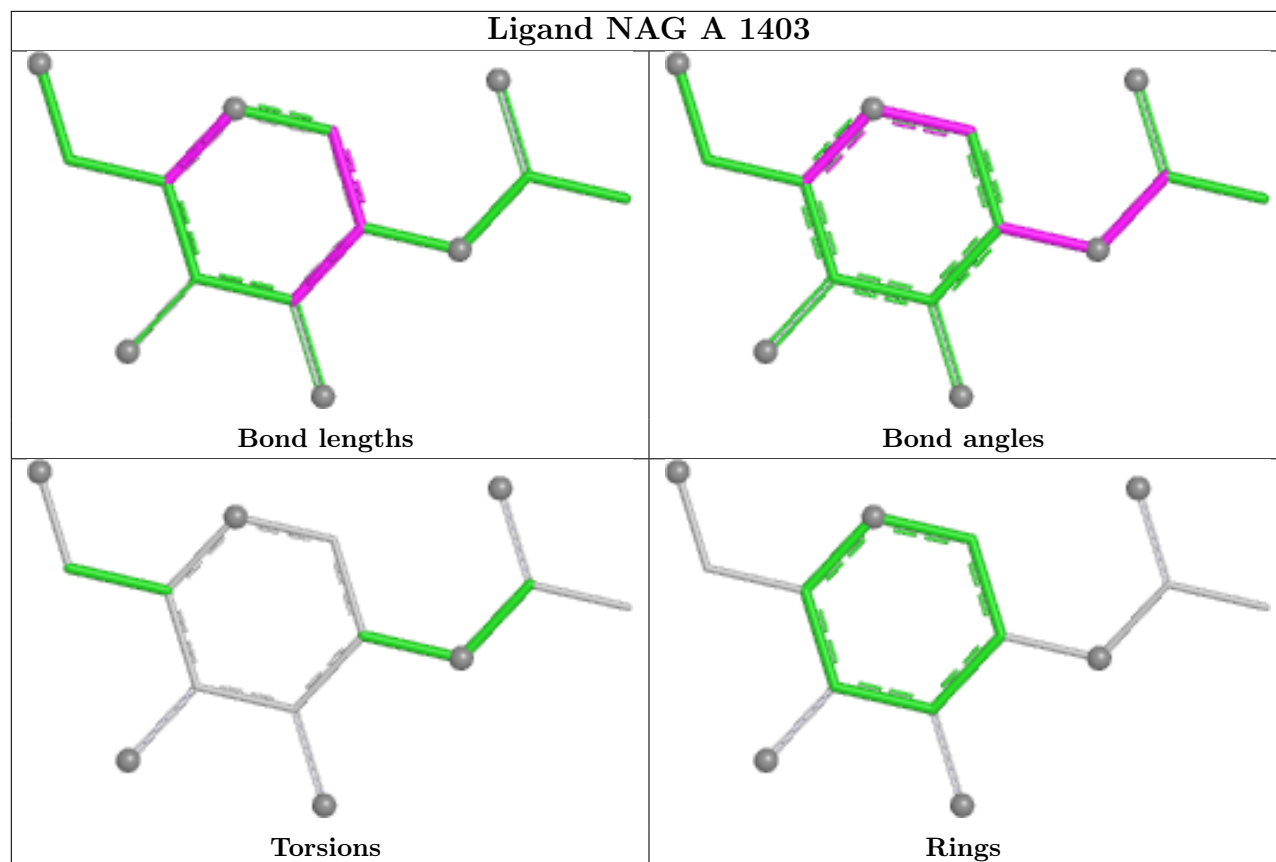
Ligand NAG C 1407



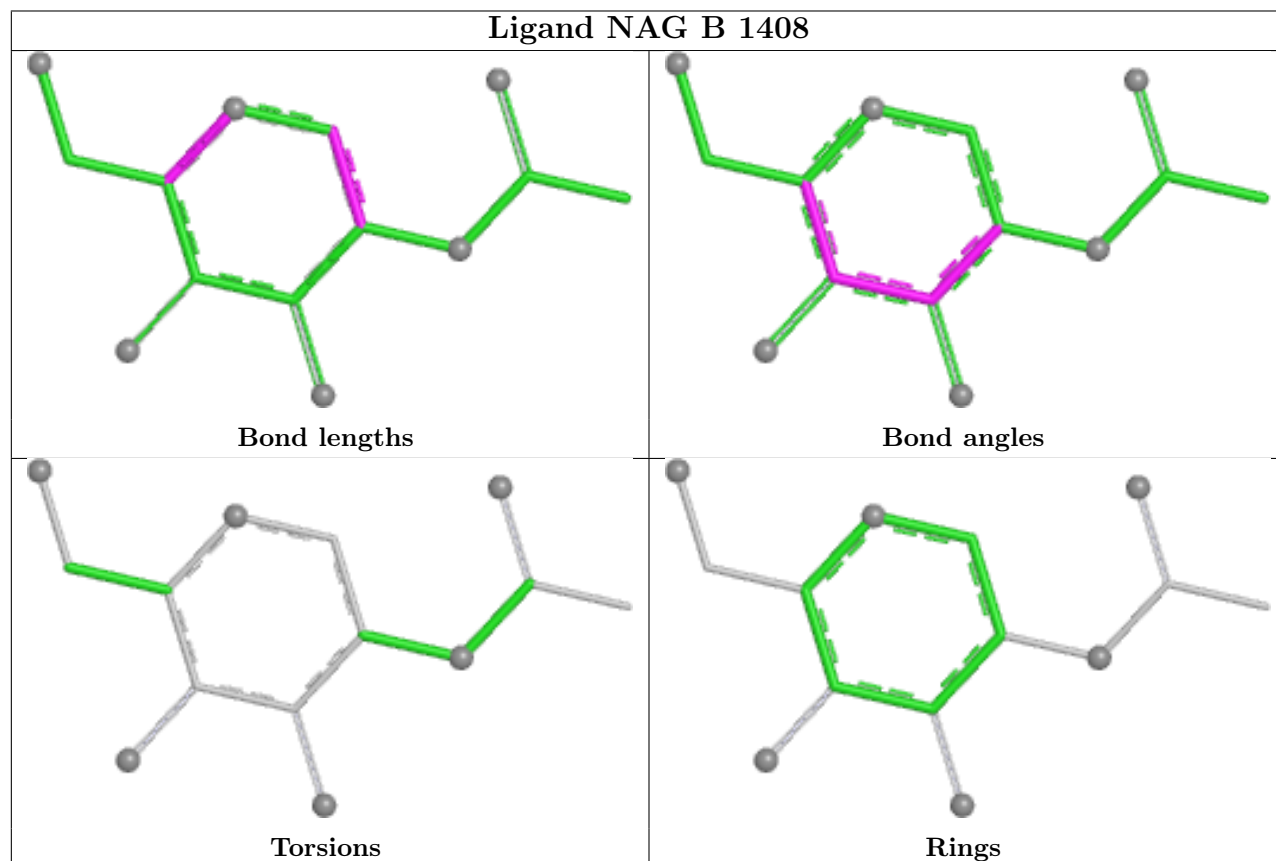
Ligand NAG A 1411

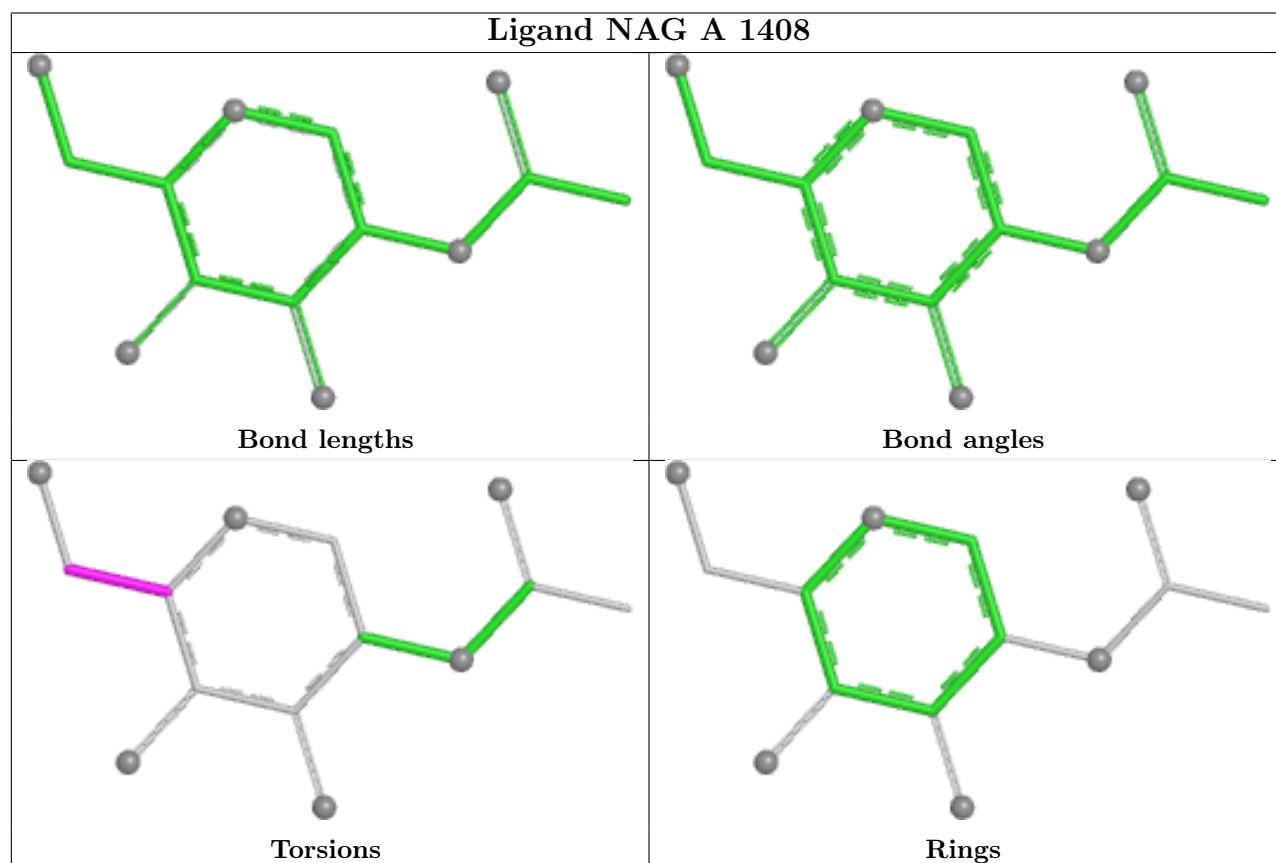
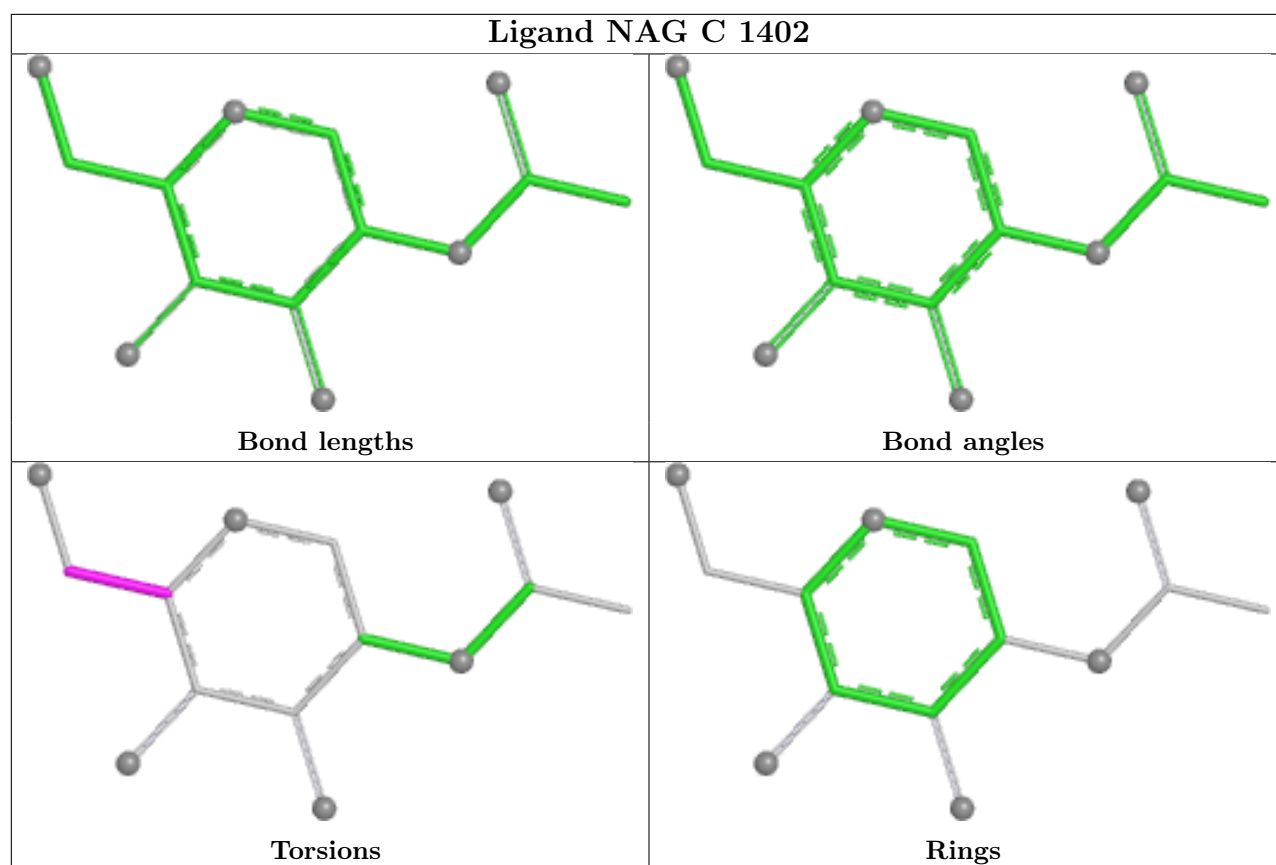


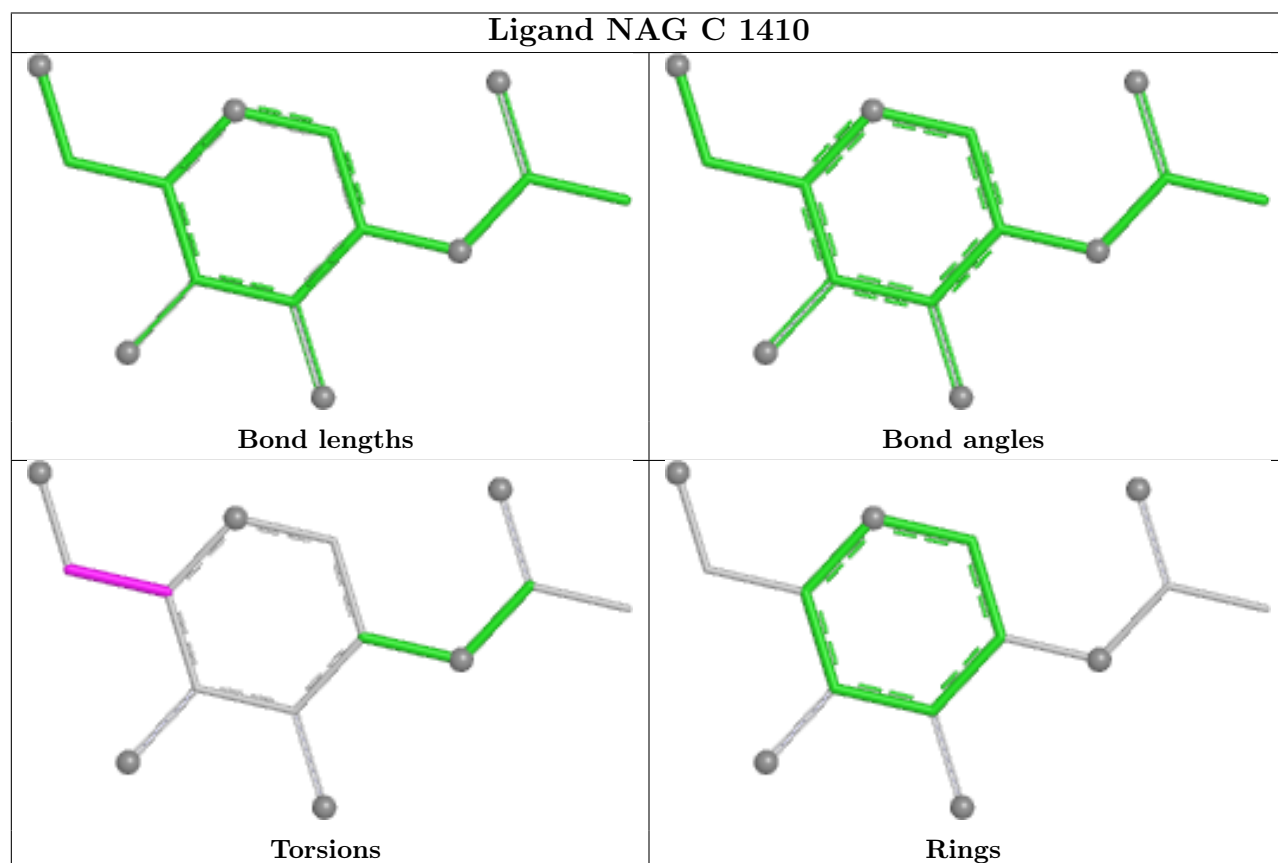
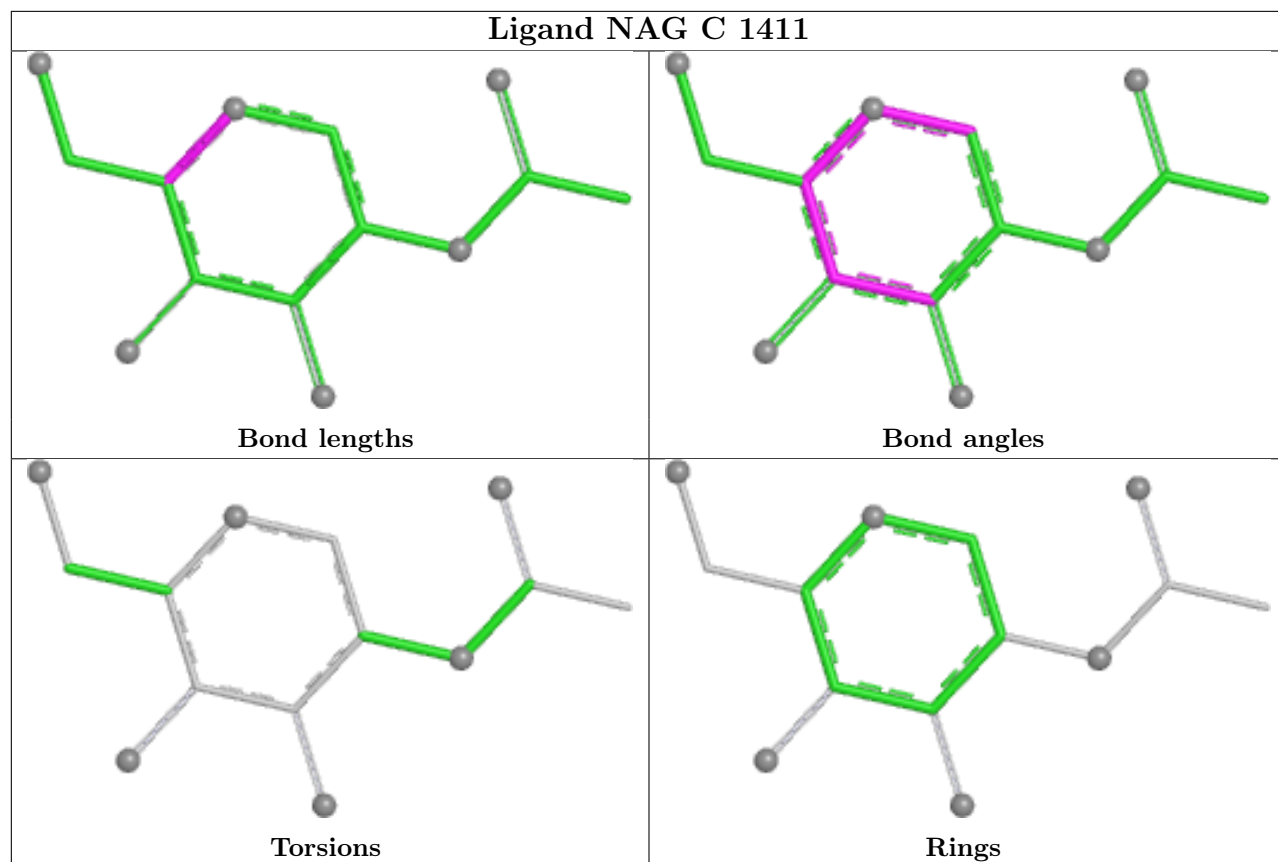
Ligand NAG A 1403



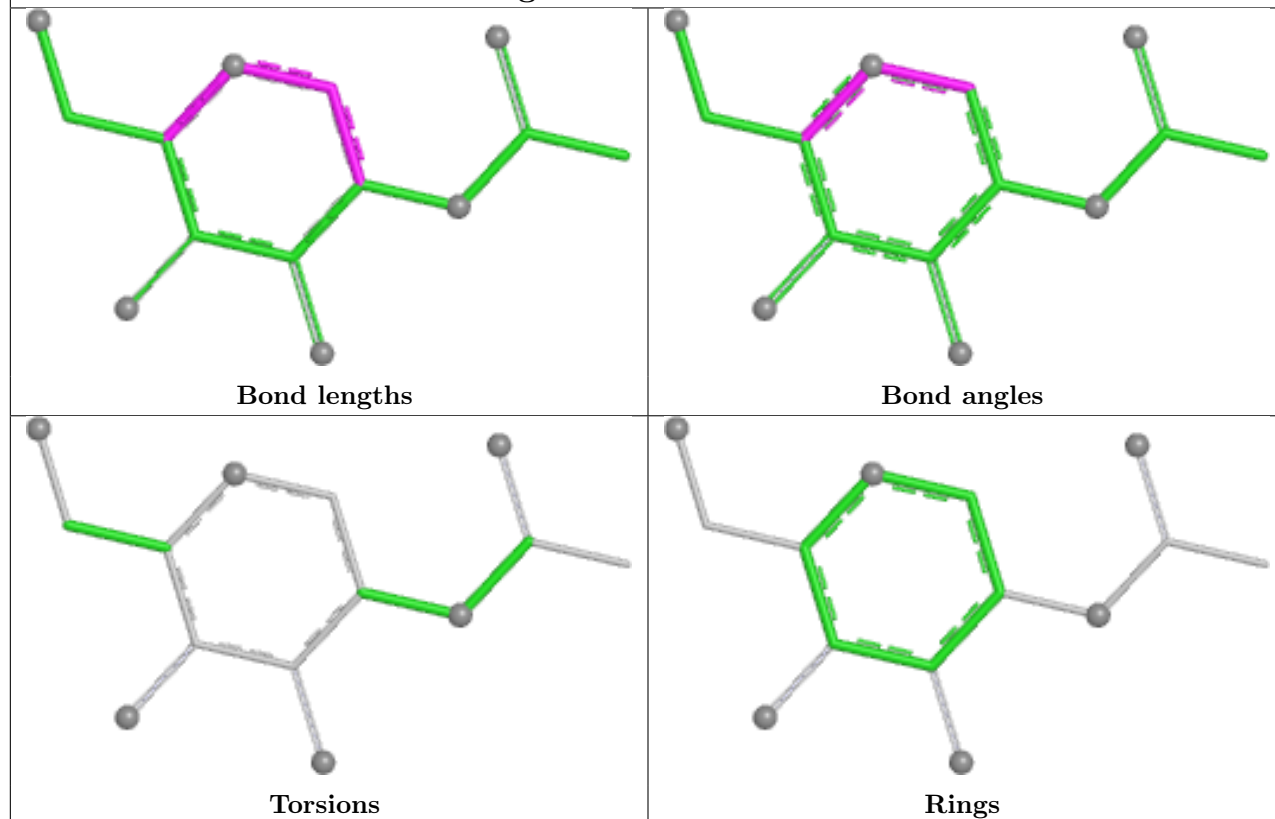
Ligand NAG B 1408



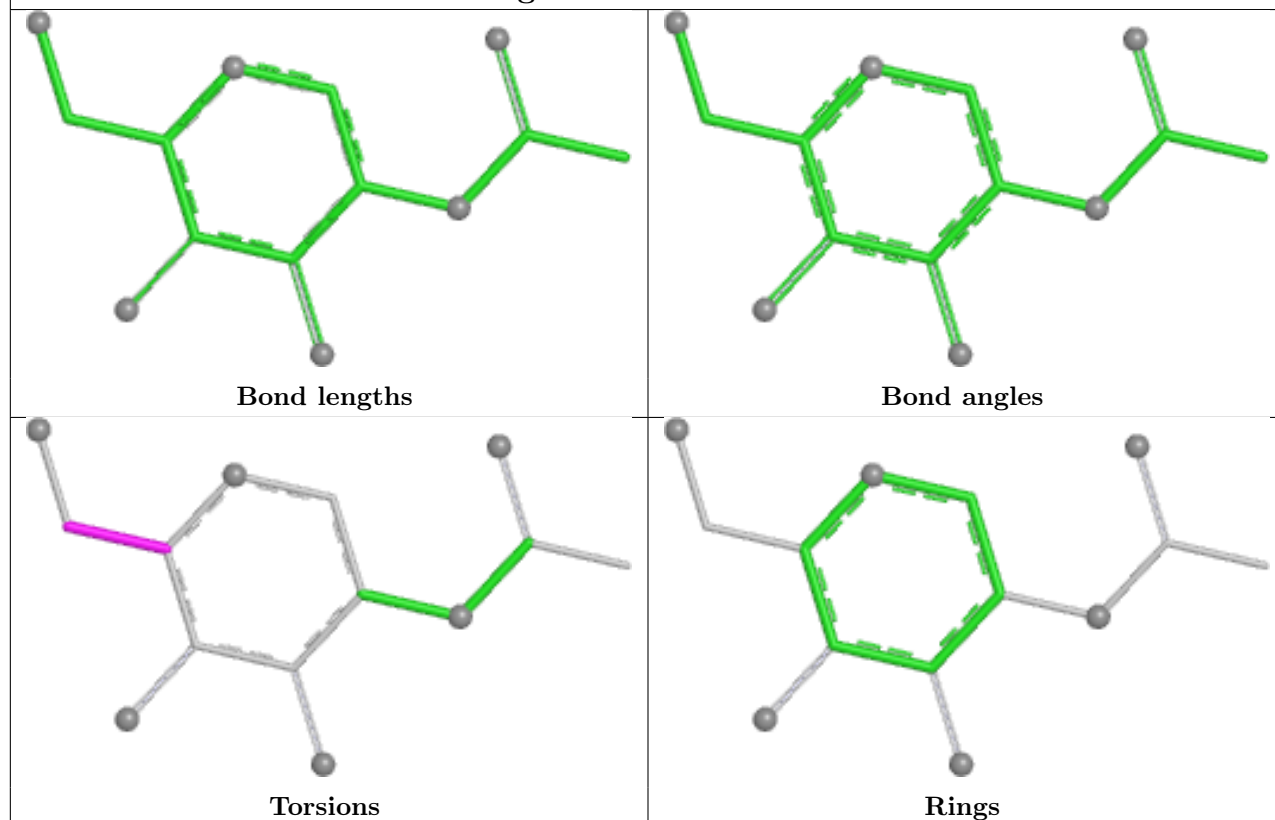




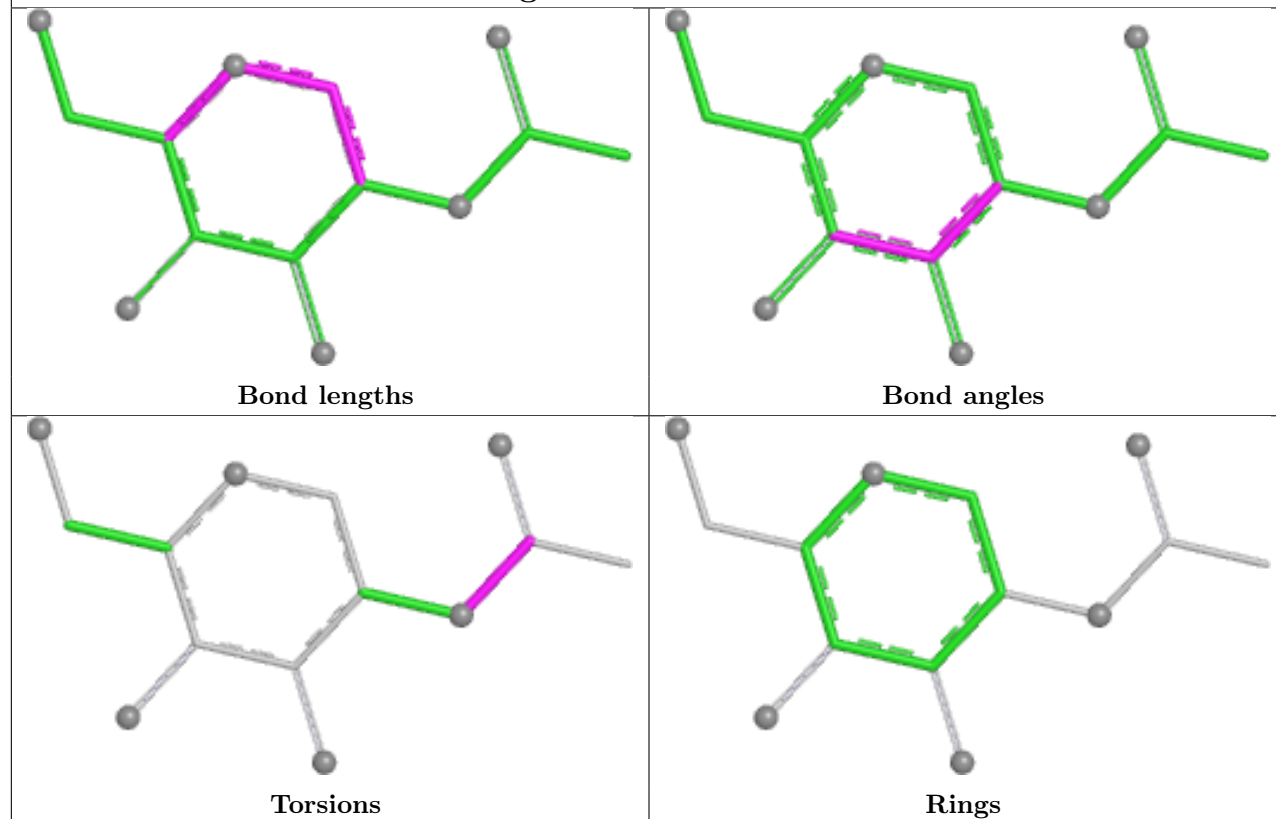
Ligand NAG C 1408



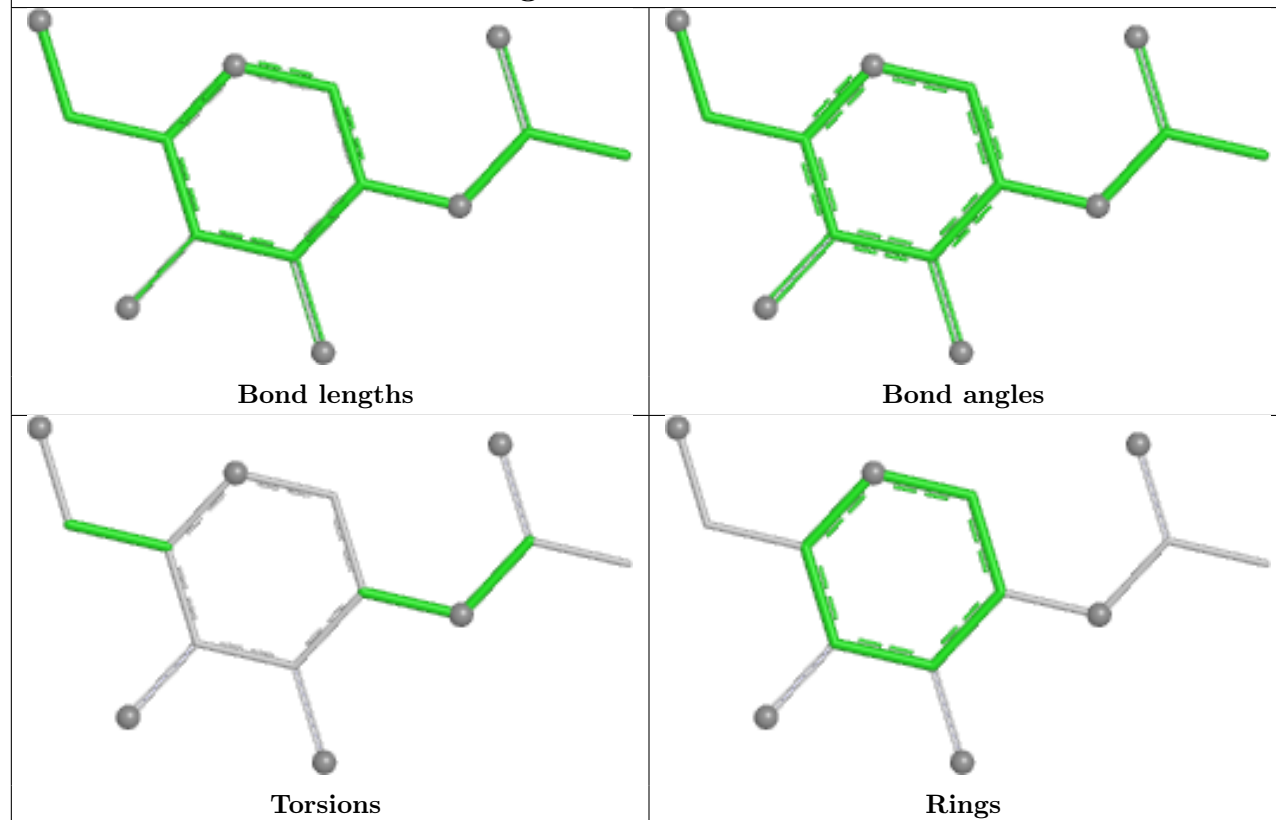
Ligand NAG A 1401



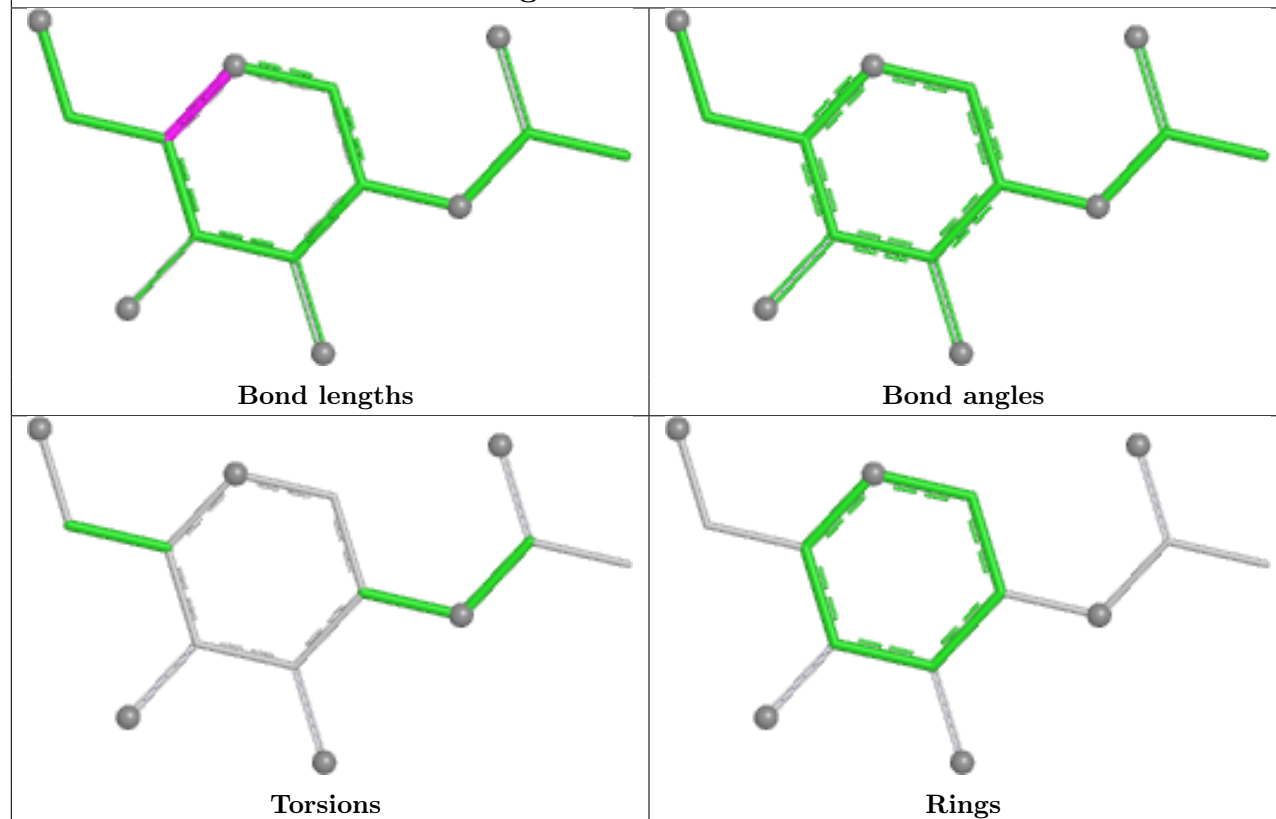
Ligand NAG B 1404



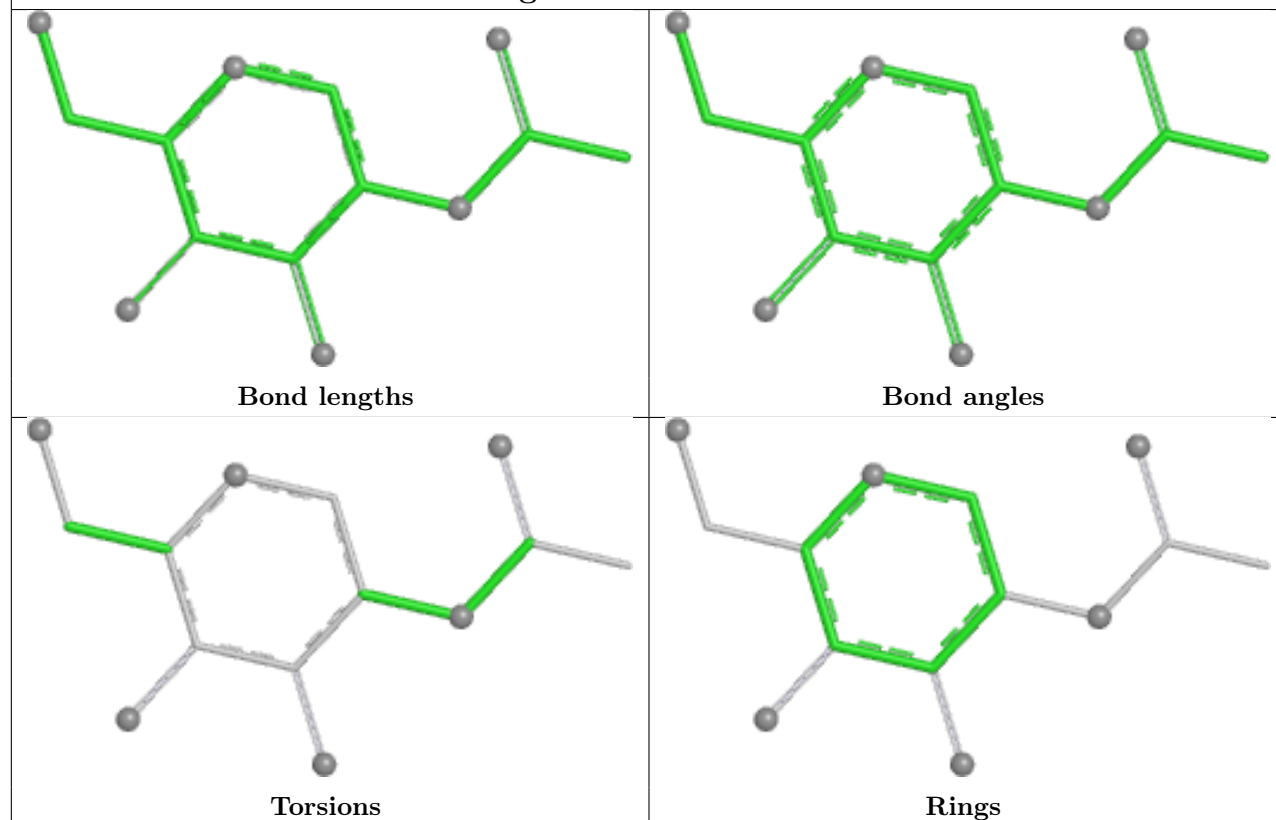
Ligand NAG C 1405



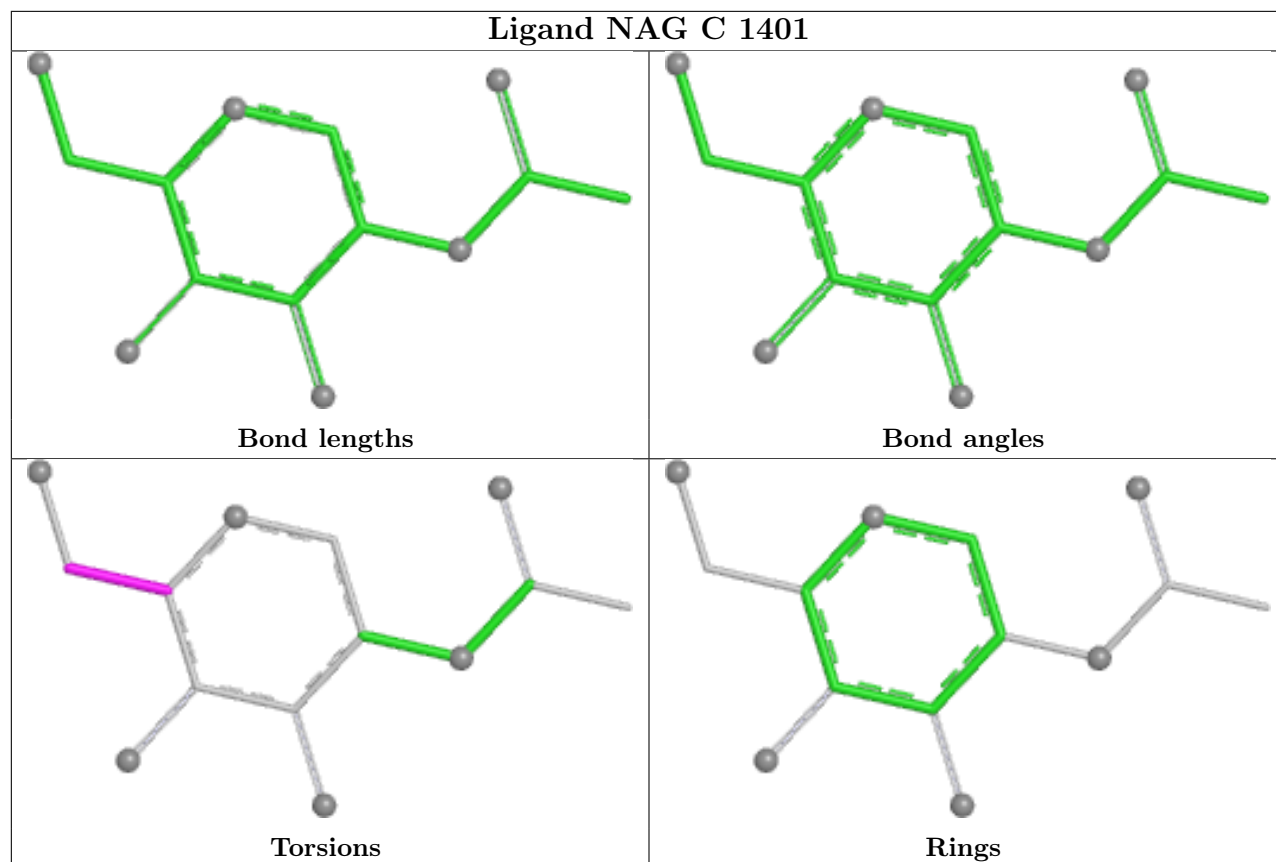
Ligand NAG B 1407



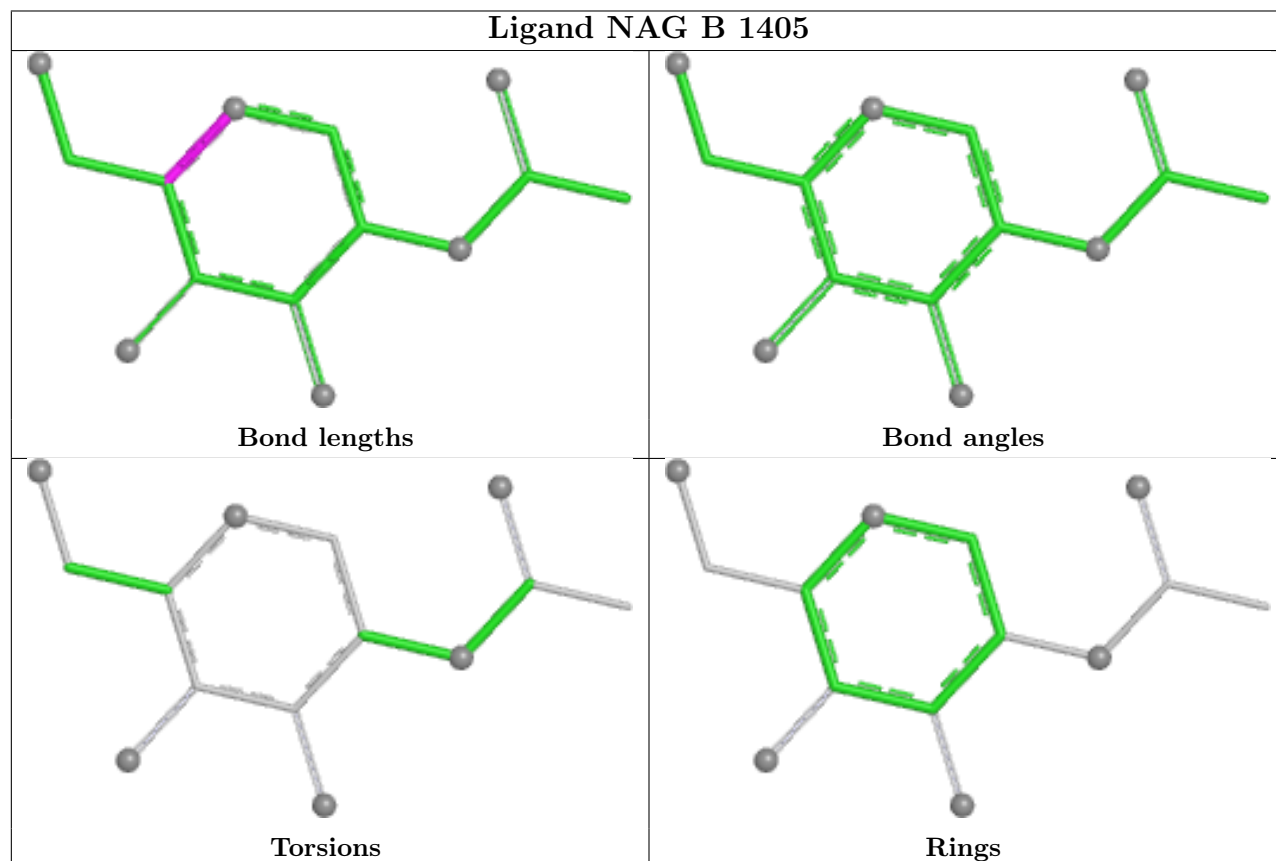
Ligand NAG C 1403



Ligand NAG C 1401



Ligand NAG B 1405



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.

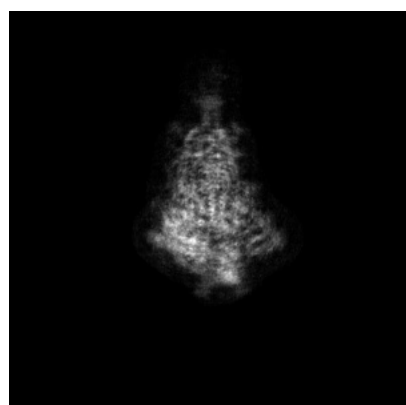
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24127. These allow visual inspection of the internal detail of the map and identification of artifacts.

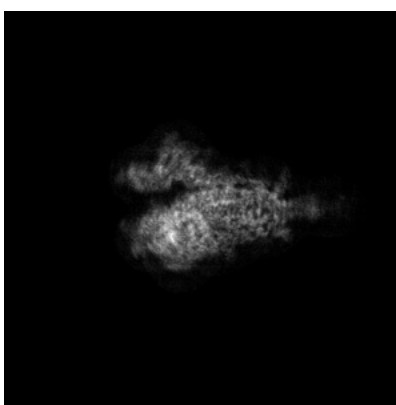
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

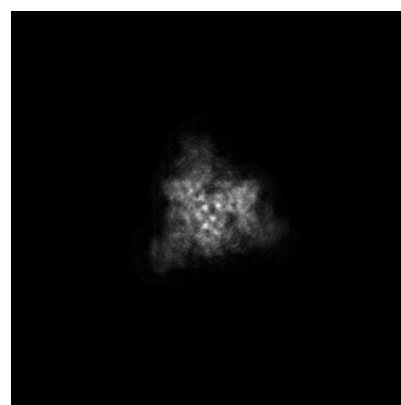
6.1.1 Primary map



X



Y

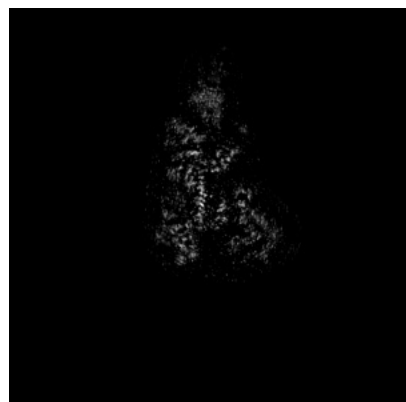


Z

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

6.2 Central slices [i](#)

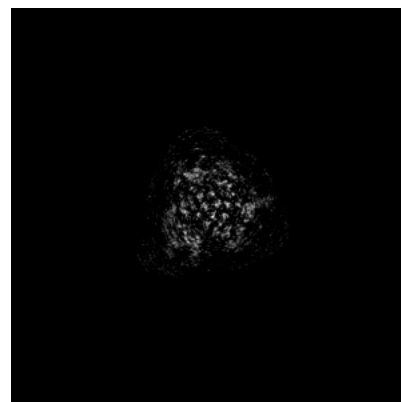
6.2.1 Primary map



X Index: 240



Y Index: 240

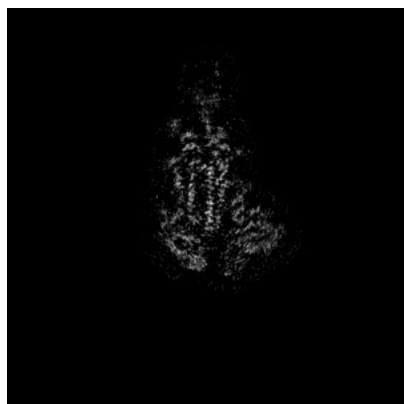


Z Index: 240

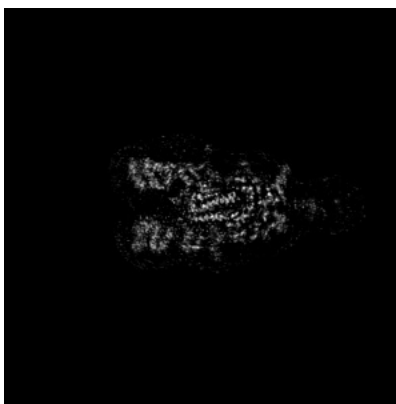
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

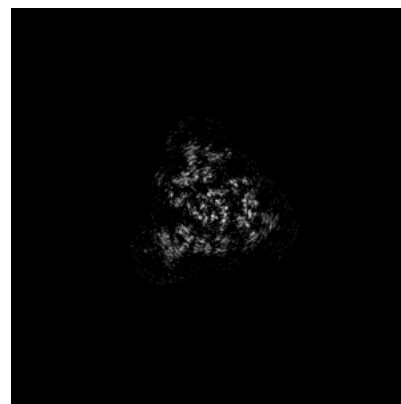
6.3.1 Primary map



X Index: 231



Y Index: 256

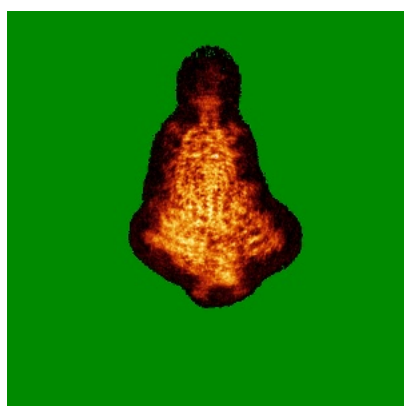


Z Index: 226

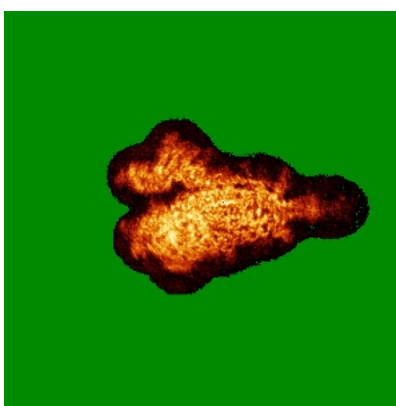
The images above show the largest variance slices of the map in three orthogonal directions.

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

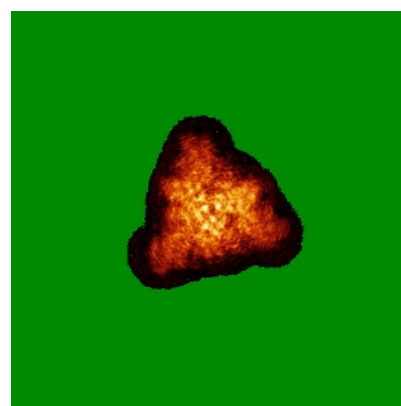
6.4.1 Primary map



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

This section was not generated.

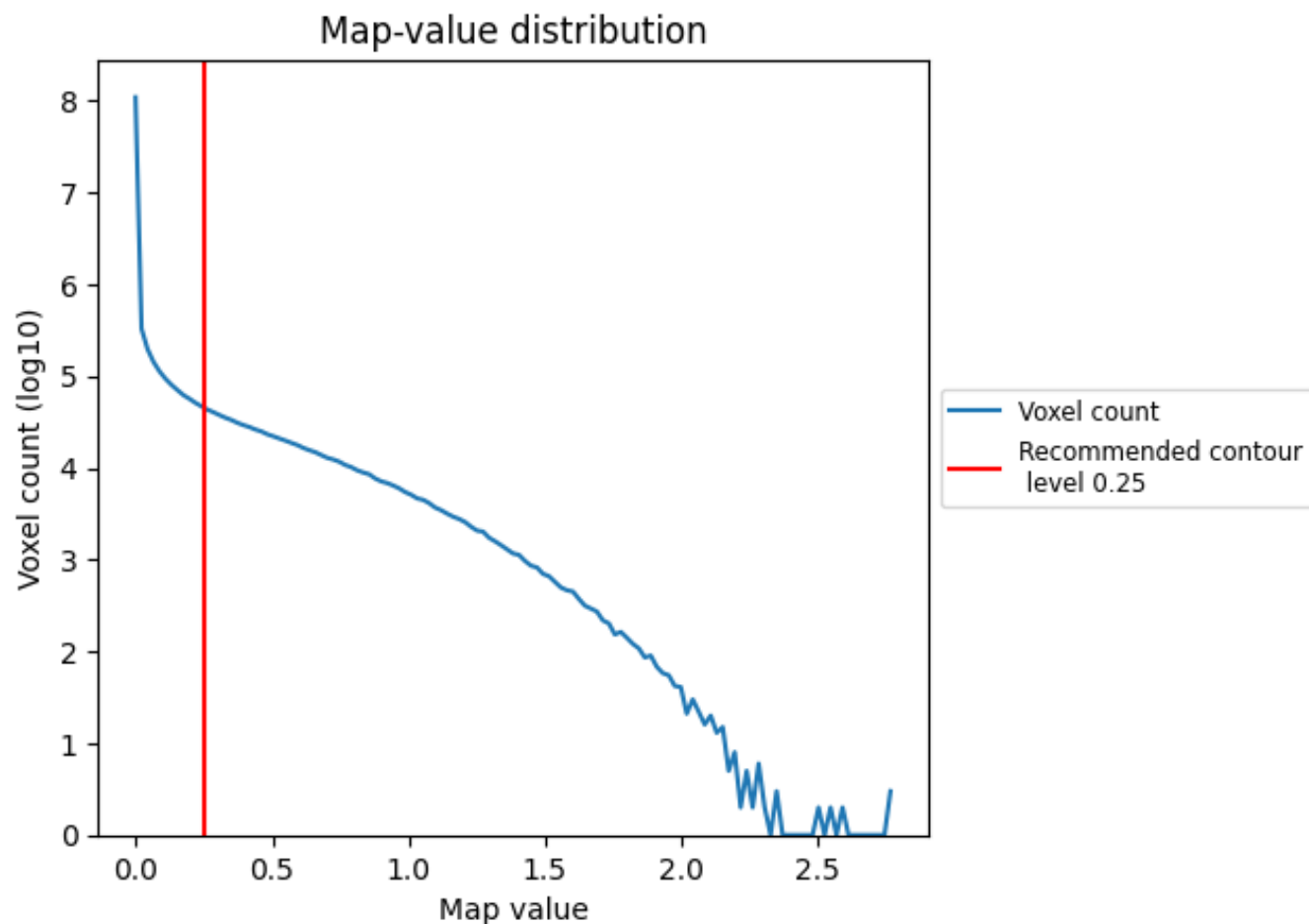
6.6 Mask visualisation

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

7 Map analysis [i](#)

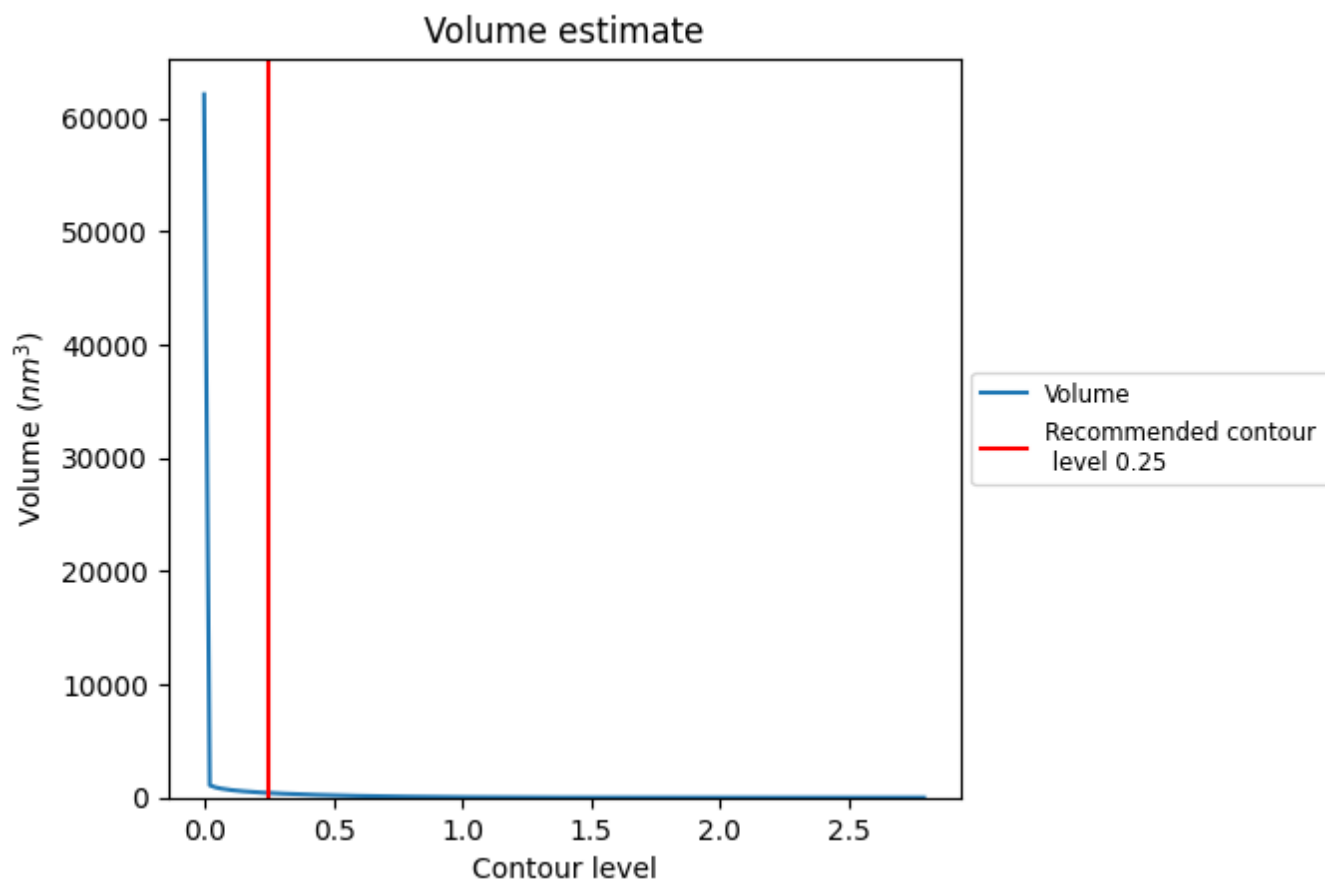
This section contains the results of statistical analysis of the map.

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.

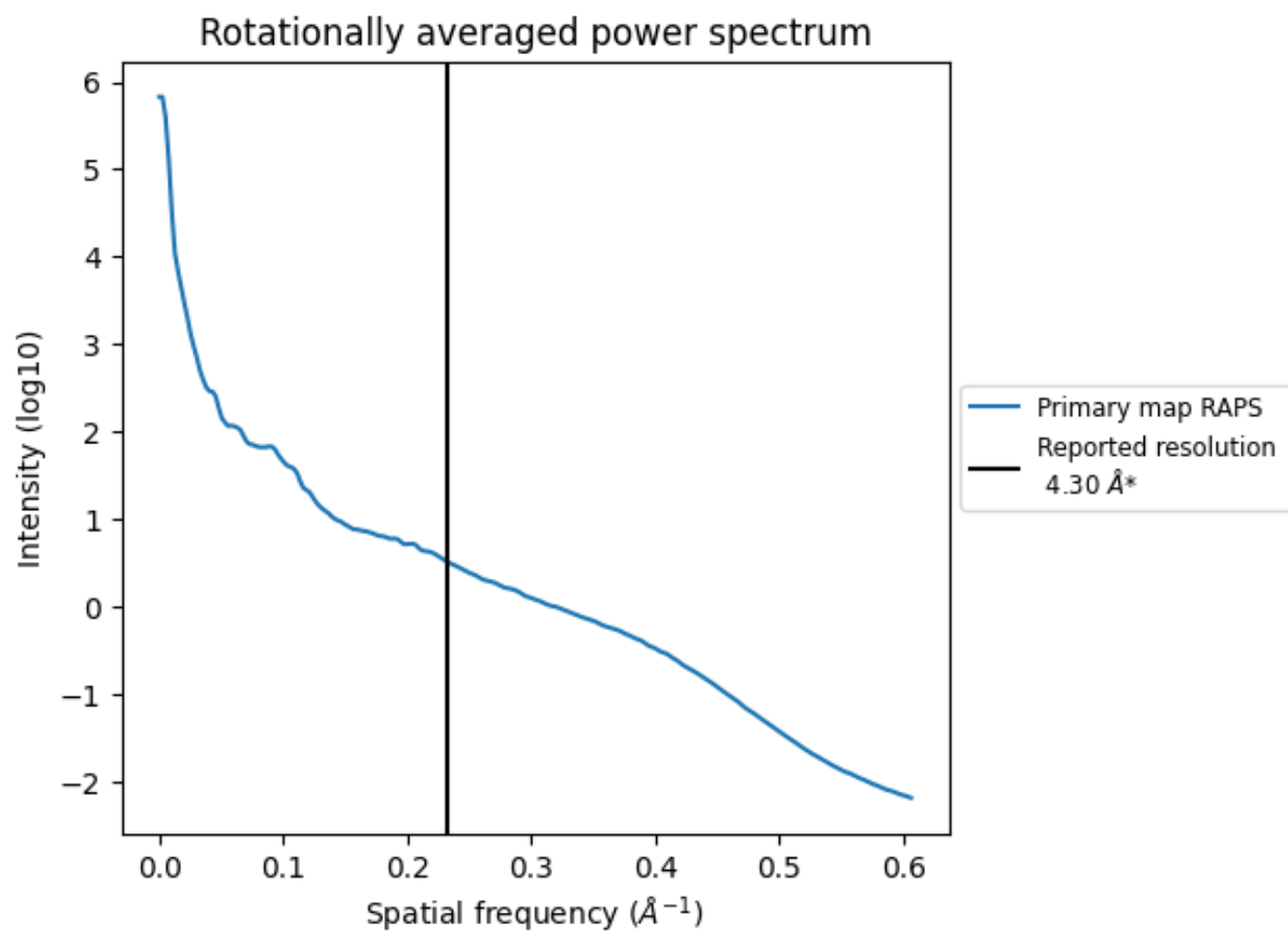
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 405 nm³; this corresponds to an approximate mass of 366 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 0.233 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

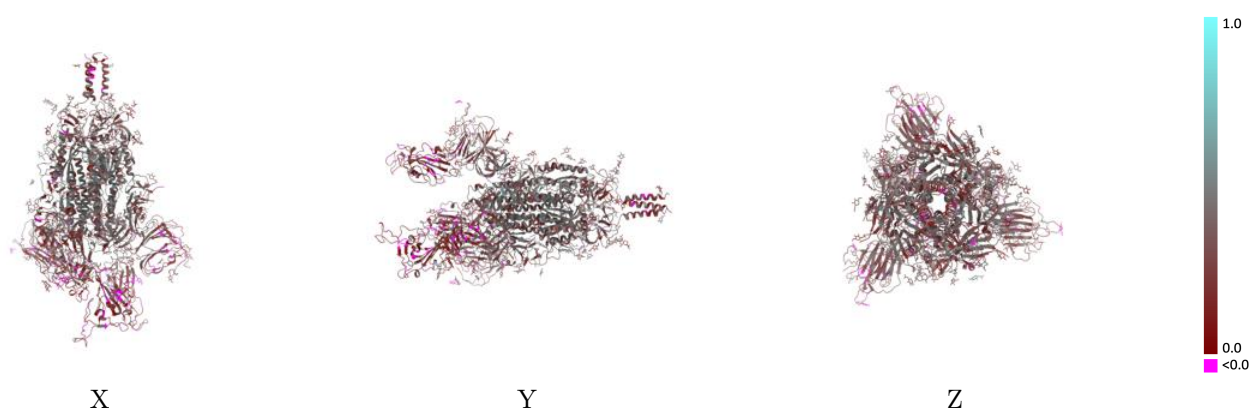
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24127 and PDB model 7N1Y. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)

This section was not generated.

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

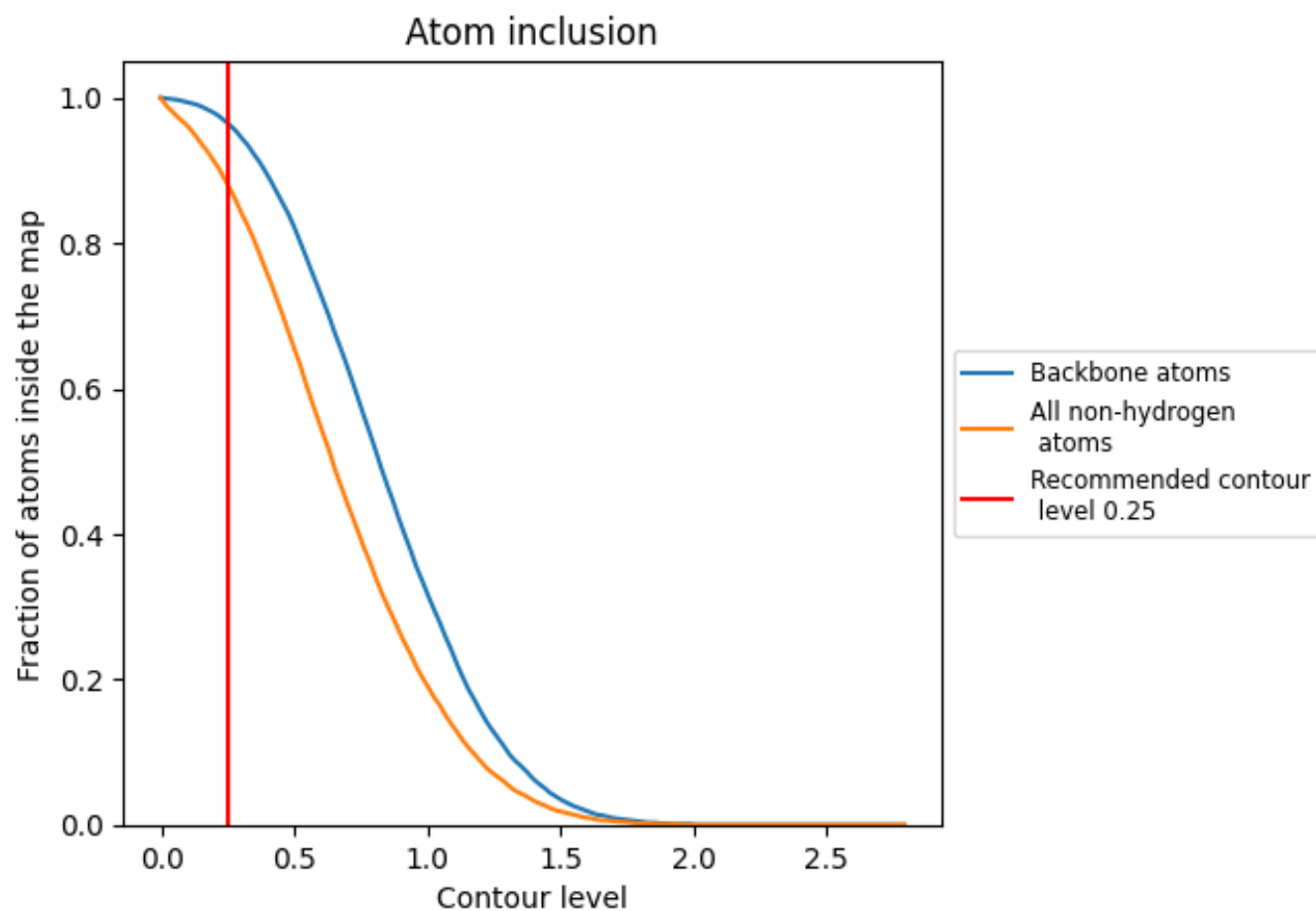


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8810	 0.3210
A	 0.8830	 0.3160
B	 0.8790	 0.3280
C	 0.8800	 0.3180
D	 0.9640	 0.3010
E	 1.0000	 0.3690
F	 0.9290	 0.2180
G	 0.7860	 0.2930
H	 0.9640	 0.4370
I	 0.6320	 0.2510
J	 0.8720	 0.1230
K	 1.0000	 0.3190
L	 0.9290	 0.2310
M	 0.7860	 0.2080
N	 0.8210	 0.2300
O	 0.8930	 0.3780
P	 0.8570	 0.3390
Q	 0.9640	 0.3740
R	 0.6840	 0.3170
S	 0.9740	 0.3770
T	 0.9740	 0.3720
U	 0.6070	 -0.0250
V	 1.0000	 0.3450
W	 0.7860	 0.2820
X	 0.9290	 0.4400
Y	 0.9290	 0.4360
Z	 0.8680	 0.3810
a	 0.9490	 0.2590
b	 0.9490	 0.3290

