



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 9, 2022 – 12:27 PM JST

PDB ID : 7XOI
Title : Aspergillus sojae alpha-glucosidase AsojAgdL in complex with trehalose
Authors : Tonozuka, T.
Deposited on : 2022-05-01
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

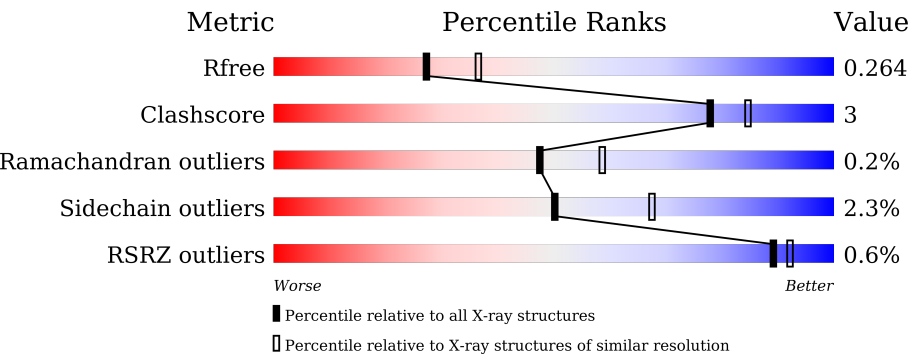
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.













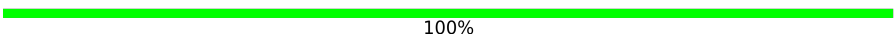


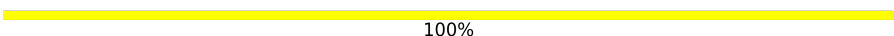

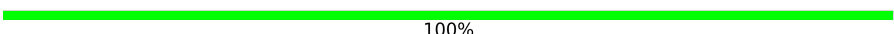
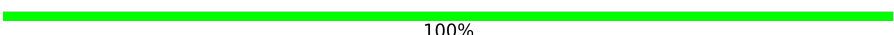
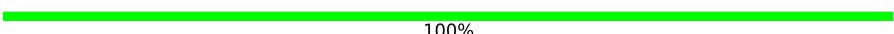
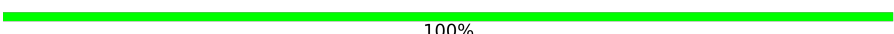

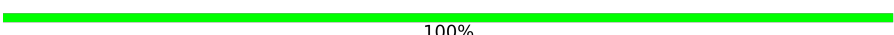
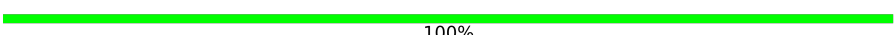
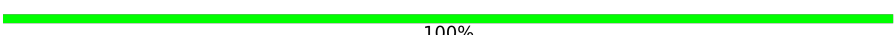
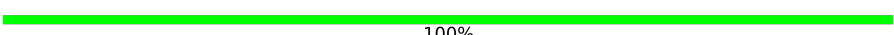
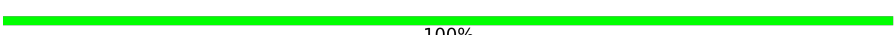
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	
1	C	548	
1	E	548	
1	G	548	
1	I	548	
1	K	548	
















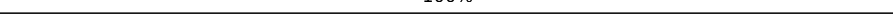

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Mol	Chain	Length	Quality of chain
1	M	548	
1	O	548	
2	B	445	
2	D	445	
2	F	445	
2	H	445	
2	J	445	
2	L	445	
2	N	445	
2	P	445	
3	Q	2	
3	S	2	
3	U	2	
3	W	2	
3	Y	2	
3	a	2	
3	c	2	
3	e	2	
3	g	2	
3	i	2	
3	k	2	
3	m	2	
3	o	2	
3	q	2	
3	s	2	

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Mol	Chain	Length	Quality of chain
3	u	2	 100%
4	R	2	 50% 50%
4	V	2	 50% 50%
4	Z	2	 100%
4	d	2	 50% 50%
4	h	2	 100%
4	l	2	 50% 50%
4	p	2	 50% 50%
4	t	2	 100%
5	T	3	 100%
5	X	3	 100%
5	b	3	 100%
5	f	3	 33% 67%
5	j	3	 67% 33%
5	n	3	 100%
5	r	3	 33% 67%
5	v	3	 67% 33%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60933 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 alpha-glucosidase N-terminal polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3747	2406	609	721	11			
1	C	465	Total	C	N	O	S	0	0	0
			3747	2406	609	721	11			
1	E	465	Total	C	N	O	S	0	0	0
			3747	2406	609	721	11			
1	G	465	Total	C	N	O	S	0	0	0
			3747	2406	609	721	11			
1	I	465	Total	C	N	O	S	0	0	0
			3747	2406	609	721	11			
1	K	465	Total	C	N	O	S	0	0	0
			3747	2406	609	721	11			
1	M	465	Total	C	N	O	S	0	0	0
			3747	2406	609	721	11			
1	O	465	Total	C	N	O	S	0	0	0
			3747	2406	609	721	11			

- Molecule 2 is a protein called alpha-glucosidase C-terminal polypeptide.

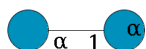
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	436	Total	C	N	O	S	0	0	0
			3397	2151	575	662	9			
2	D	436	Total	C	N	O	S	0	0	0
			3397	2151	575	662	9			
2	F	436	Total	C	N	O	S	0	0	0
			3397	2151	575	662	9			
2	H	436	Total	C	N	O	S	0	0	0
			3397	2151	575	662	9			
2	J	436	Total	C	N	O	S	0	0	0
			3397	2151	575	662	9			
2	L	436	Total	C	N	O	S	0	0	0
			3397	2151	575	662	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	436	Total	C	N	O	S	0	0	0
			3397	2151	575	662	9			
2	P	436	Total	C	N	O	S	0	0	0
			3397	2151	575	662	9			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	Q	2	Total	C	O	0	0	0
			23	12	11			
3	S	2	Total	C	O	0	0	0
			23	12	11			
3	U	2	Total	C	O	0	0	0
			23	12	11			
3	W	2	Total	C	O	0	0	0
			23	12	11			
3	Y	2	Total	C	O	0	0	0
			23	12	11			
3	a	2	Total	C	O	0	0	0
			23	12	11			
3	c	2	Total	C	O	0	0	0
			23	12	11			
3	e	2	Total	C	O	0	0	0
			23	12	11			
3	g	2	Total	C	O	0	0	0
			23	12	11			
3	i	2	Total	C	O	0	0	0
			23	12	11			
3	k	2	Total	C	O	0	0	0
			23	12	11			
3	m	2	Total	C	O	0	0	0
			23	12	11			
3	o	2	Total	C	O	0	0	0
			23	12	11			
3	q	2	Total	C	O	0	0	0
			23	12	11			
3	s	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	u	2	Total	C	O	0	0	0
			23	12	11			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	h	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	l	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	p	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	t	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



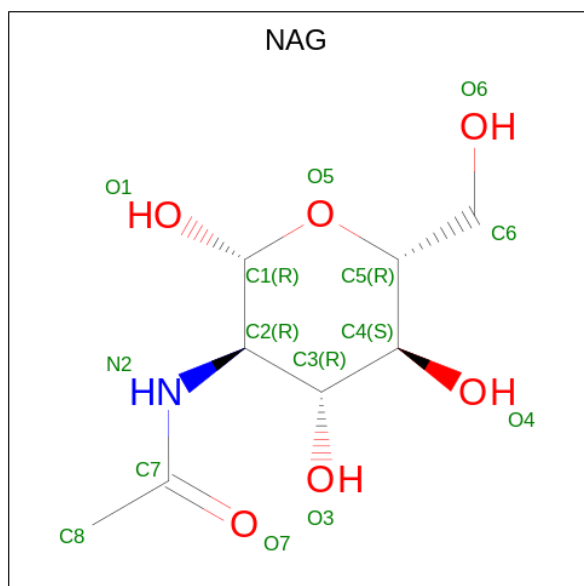
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	T	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	b	3	Total	C	N	O	0	0	0
			39	22	2	15			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	f	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	j	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	n	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	r	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	v	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		
6	M	1	Total	C	N	O	0	0
			14	8	1	5		
6	M	1	Total	C	N	O	0	0
			14	8	1	5		
6	M	1	Total	C	N	O	0	0
			14	8	1	5		
6	M	1	Total	C	N	O	0	0
			14	8	1	5		

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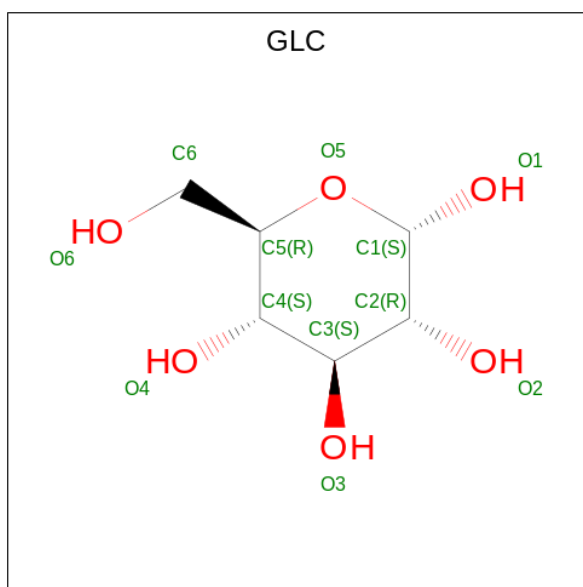
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	N	1	Total	C	N	O	0	0
			14	8	1	5		
6	N	1	Total	C	N	O	0	0
			14	8	1	5		
6	O	1	Total	C	N	O	0	0
			14	8	1	5		
6	O	1	Total	C	N	O	0	0
			14	8	1	5		
6	O	1	Total	C	N	O	0	0
			14	8	1	5		
6	O	1	Total	C	N	O	0	0
	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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		
7	D	1	Total	Na	0	0
			1	1		
7	F	1	Total	Na	0	0
			1	1		
7	H	1	Total	Na	0	0
			1	1		
7	J	1	Total	Na	0	0
			1	1		
7	L	1	Total	Na	0	0
			1	1		
7	N	1	Total	Na	0	0
			1	1		
7	P	1	Total	Na	0	0
			1	1		

- Molecule 8 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			12	6	6		
8	C	1	Total	C	O	0	0
			12	6	6		
8	E	1	Total	C	O	0	0
			12	6	6		
8	G	1	Total	C	O	0	0
			12	6	6		
8	I	1	Total	C	O	0	0
			12	6	6		
8	L	1	Total	C	O	0	0
			12	6	6		
8	M	1	Total	C	O	0	0
			12	6	6		
8	P	1	Total	C	O	0	0
			12	6	6		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	148	Total	O	0	0
			148	148		
9	B	124	Total	O	0	0
			124	124		
9	C	117	Total	O	0	0
			117	117		
9	D	103	Total	O	0	0
			103	103		

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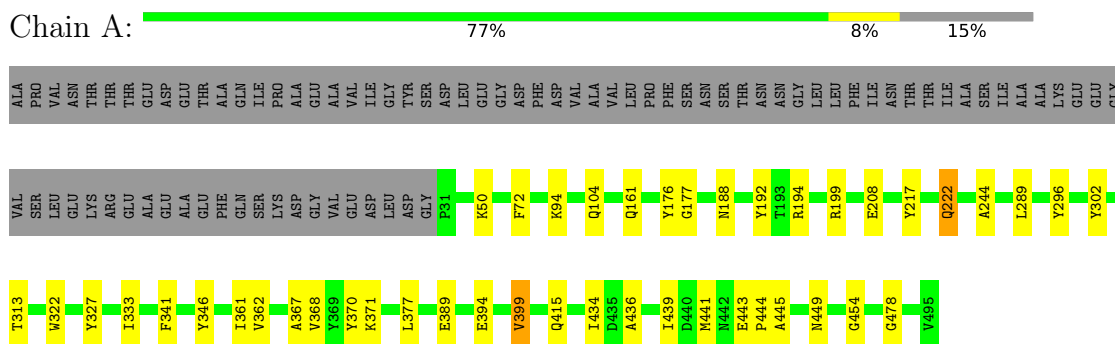
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	138	Total 138	O 138	0	0
9	F	128	Total 128	O 128	0	0
9	G	145	Total 145	O 145	0	0
9	H	114	Total 114	O 114	0	0
9	I	143	Total 143	O 143	0	0
9	J	105	Total 105	O 105	0	0
9	K	138	Total 138	O 138	0	0
9	L	101	Total 101	O 101	0	0
9	M	147	Total 147	O 147	0	0
9	N	117	Total 117	O 117	0	0
9	O	105	Total 105	O 105	0	0
9	P	102	Total 102	O 102	0	0

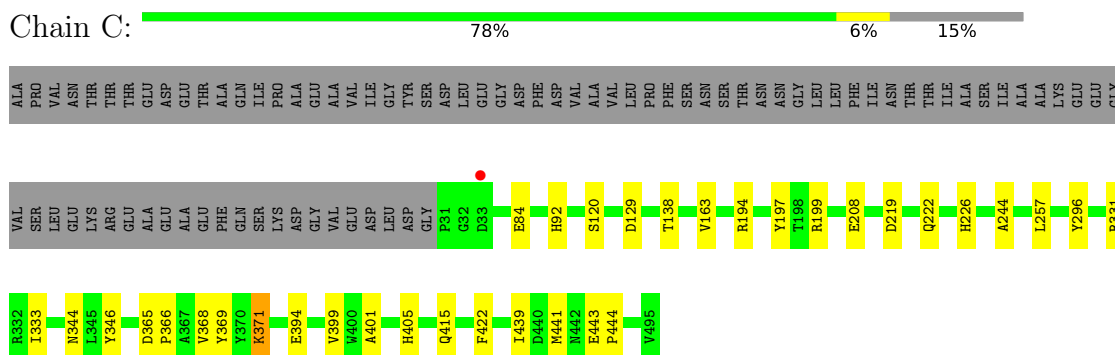
3 Residue-property plots

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

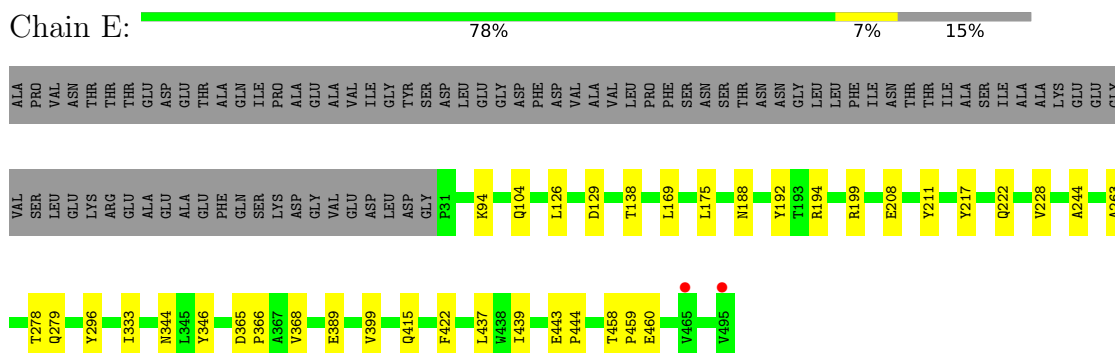
- Molecule 1: alpha-glucosidase N-terminal polypeptide



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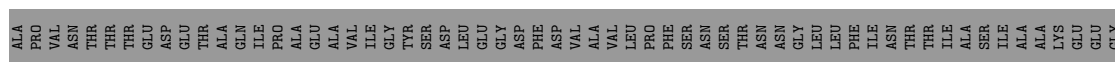
- Molecule 1: alpha-glucosidase N-terminal polypeptide





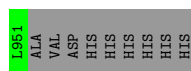
- Molecule 1: alpha-glucosidase N-terminal polypeptide

Chain O: 78% 7% 15%



- Molecule 2: alpha-glucosidase C-terminal polypeptide

Chain B: 91% 6% .



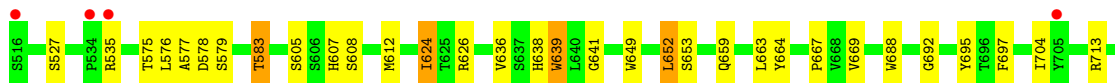
- Molecule 2: alpha-glucosidase C-terminal polypeptide

Chain D: 89% 9% .

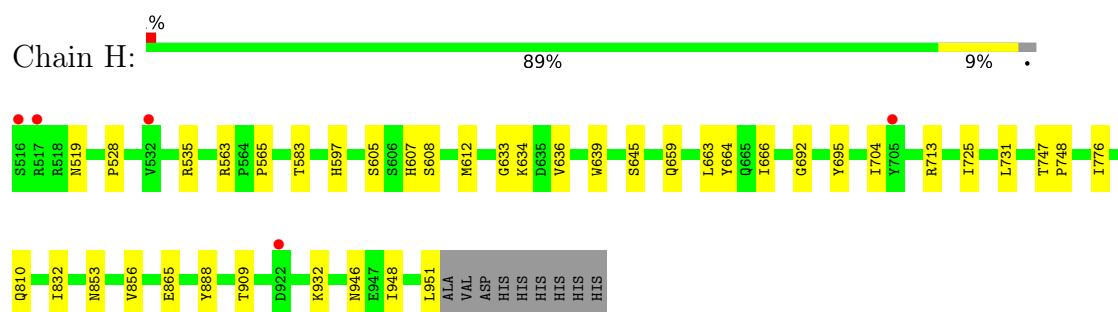


- Molecule 2: alpha-glucosidase C-terminal polypeptide

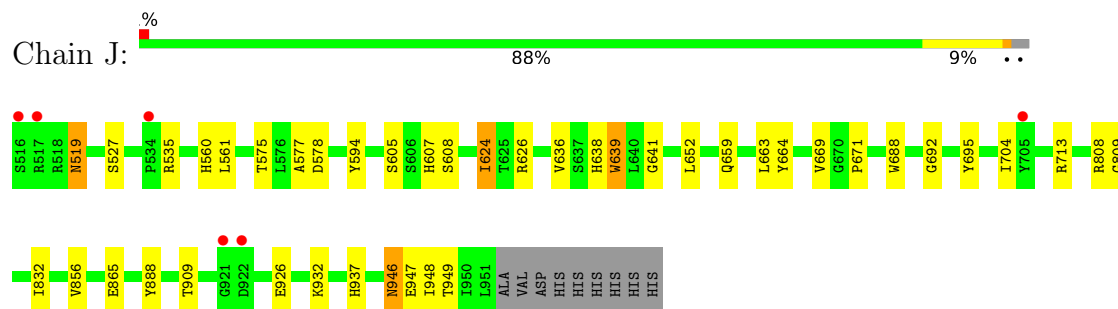
Chain F: 88% 9% ..



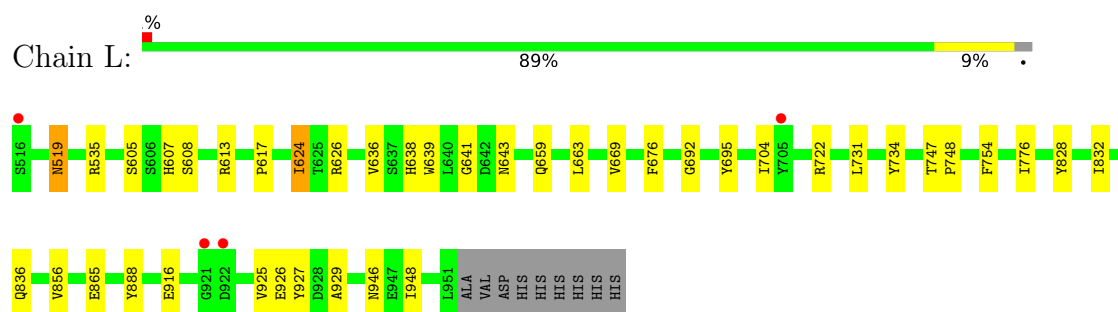
- Molecule 2: alpha-glucosidase C-terminal polypeptide



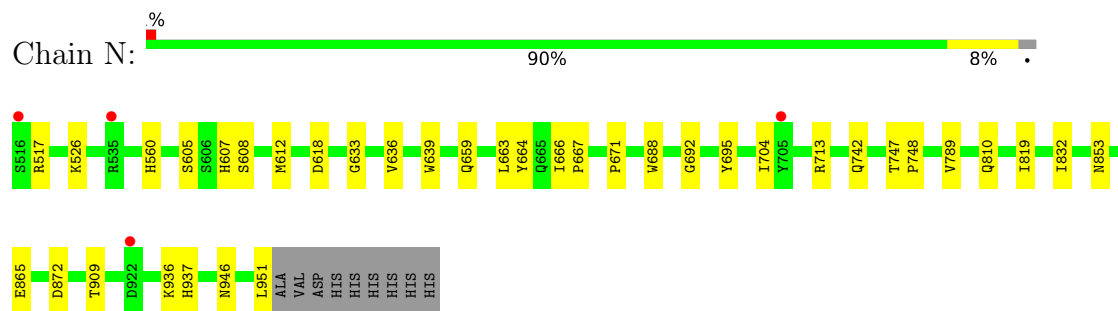
- Molecule 2: alpha-glucosidase C-terminal polypeptide



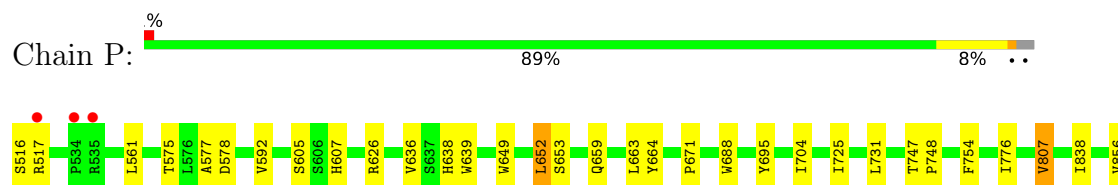
- Molecule 2: alpha-glucosidase C-terminal polypeptide



- Molecule 2: alpha-glucosidase C-terminal polypeptide



- Molecule 2: alpha-glucosidase C-terminal polypeptide





- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain Q: 100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain S: 100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain U: 100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain W: 100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain Y: 100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain a: 100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain c: 100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain e:  100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain g:  100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain i:  50% 50%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain k:  100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain m:  100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain o:  100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain q:  100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain s:  100%



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain u:  100%



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

Chain R:  50%  50%



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

Chain V:  50%  50%



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

Chain Z:  100%



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

Chain d:  50%  50%




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

Chain h:  100%



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

Chain l:  50% 50%

NAG1
NAG2

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

Chain p:  50% 50%

NAG1
NAG2

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

Chain t:  100%

NAG1
NAG2

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

Chain T:  100%

NAG1
NAG2
BMA3

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

Chain X:  100%

NAG1
NAG2
BMA3

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

Chain b:  100%

NAG1
NAG2
BMA3

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

Chain f:  33% 67%

NAG1
NAG2
BMA3

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

Chain j:  67% 33%

MAG1
MAG2
BMA3

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

Chain n:  100%

MAG1
MAG2
BMA3

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

Chain r:  33% 67%

MAG1
MAG2
BMA3

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

Chain v:  67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.33Å 106.04Å 206.37Å 90.58° 90.06° 92.20°	Depositor
Resolution (Å)	49.14 – 2.30 49.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.14-2.30) 97.3 (49.09-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.227 , 0.267 0.223 , 0.264	Depositor DCC
R_{free} test set	16975 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 14.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l 0.140 for -h,k,-l 0.109 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	60933	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4611e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.62	0/3875	0.73	0/5306
1	C	0.62	0/3875	0.72	0/5306
1	E	0.62	0/3875	0.73	0/5306
1	G	0.62	0/3875	0.73	0/5306
1	I	0.62	0/3875	0.73	0/5306
1	K	0.62	0/3875	0.71	0/5306
1	M	0.62	0/3875	0.72	0/5306
1	O	0.62	0/3875	0.72	0/5306
2	B	0.64	0/3487	0.73	0/4755
2	D	0.65	0/3487	0.73	0/4755
2	F	0.64	0/3487	0.74	0/4755
2	H	0.64	0/3487	0.73	0/4755
2	J	0.65	0/3487	0.73	0/4755
2	L	0.64	0/3487	0.73	0/4755
2	N	0.65	0/3487	0.73	0/4755
2	P	0.65	0/3487	0.73	0/4755
All	All	0.63	0/58896	0.73	0/80488

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3747	0	3459	28	0
1	C	3747	0	3459	18	0
1	E	3747	0	3459	23	0
1	G	3747	0	3459	32	0
1	I	3747	0	3459	21	0
1	K	3747	0	3461	22	0
1	M	3747	0	3459	27	0
1	O	3747	0	3459	21	0
2	B	3397	0	3217	18	0
2	D	3397	0	3218	23	0
2	F	3397	0	3217	33	0
2	H	3397	0	3216	22	0
2	J	3397	0	3216	30	0
2	L	3397	0	3216	26	0
2	N	3397	0	3217	22	0
2	P	3397	0	3217	22	0
3	Q	23	0	21	0	0
3	S	23	0	21	0	0
3	U	23	0	21	0	0
3	W	23	0	21	0	0
3	Y	23	0	21	0	0
3	a	23	0	21	0	0
3	c	23	0	21	0	0
3	e	23	0	21	0	0
3	g	23	0	21	0	0
3	i	23	0	21	0	0
3	k	23	0	21	0	0
3	m	23	0	21	0	0
3	o	23	0	21	0	0
3	q	23	0	21	0	0
3	s	23	0	21	0	0
3	u	23	0	21	0	0
4	R	28	0	25	0	0
4	V	28	0	25	0	0
4	Z	28	0	25	0	0
4	d	28	0	25	0	0
4	h	28	0	25	0	0
4	l	28	0	25	0	0
4	p	28	0	25	0	0
4	t	28	0	25	0	0
5	T	39	0	34	1	0
5	X	39	0	34	0	0
5	b	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	f	39	0	34	0	0
5	j	39	0	34	0	0
5	n	39	0	34	0	0
5	r	39	0	34	0	0
5	v	39	0	34	0	0
6	A	70	0	65	1	0
6	B	28	0	26	0	0
6	C	70	0	65	0	0
6	D	28	0	26	0	0
6	E	70	0	65	0	0
6	F	28	0	26	0	0
6	G	70	0	65	0	0
6	H	42	0	39	0	0
6	I	70	0	65	0	0
6	J	42	0	39	0	0
6	K	42	0	39	0	0
6	L	42	0	39	0	0
6	M	70	0	65	0	0
6	N	28	0	26	0	0
6	O	70	0	65	0	0
6	P	28	0	26	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
7	J	1	0	0	0	0
7	L	1	0	0	0	0
7	N	1	0	0	0	0
7	P	1	0	0	0	0
8	B	12	0	12	0	0
8	C	12	0	12	0	0
8	E	12	0	12	0	0
8	G	12	0	12	0	0
8	I	12	0	12	0	0
8	L	12	0	12	0	0
8	M	12	0	12	0	0
8	P	12	0	12	0	0
9	A	148	0	0	0	0
9	B	124	0	0	0	0
9	C	117	0	0	0	0
9	D	103	0	0	0	0
9	E	138	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	128	0	0	0	0
9	G	145	0	0	0	0
9	H	114	0	0	0	0
9	I	143	0	0	0	0
9	J	105	0	0	0	0
9	K	138	0	0	0	0
9	L	101	0	0	0	0
9	M	147	0	0	0	0
9	N	117	0	0	0	0
9	O	105	0	0	0	0
9	P	102	0	0	0	0
All	All	60933	0	55053	323	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 3.

The worst 5 of 323 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)
2:P:605:SER:HB3	2:P:636:VAL:HG11	1.56	0.88
2:F:575:THR:HG22	2:F:577:ALA:H	1.44	0.83
2:D:605:SER:HB3	2:D:636:VAL:HG11	1.61	0.82
2:P:575:THR:HG22	2:P:577:ALA:H	1.45	0.81
2:J:575:THR:HG22	2:J:577:ALA:H	1.47	0.79

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	463/548 (84%)	444 (96%)	18 (4%)	1 (0%)	47 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	463/548 (84%)	440 (95%)	22 (5%)	1 (0%)	47	58
1	E	463/548 (84%)	442 (96%)	20 (4%)	1 (0%)	47	58
1	G	463/548 (84%)	441 (95%)	21 (4%)	1 (0%)	47	58
1	I	463/548 (84%)	446 (96%)	17 (4%)	0	100	100
1	K	463/548 (84%)	442 (96%)	20 (4%)	1 (0%)	47	58
1	M	463/548 (84%)	440 (95%)	22 (5%)	1 (0%)	47	58
1	O	463/548 (84%)	447 (96%)	15 (3%)	1 (0%)	47	58
2	B	434/445 (98%)	413 (95%)	20 (5%)	1 (0%)	47	58
2	D	434/445 (98%)	417 (96%)	16 (4%)	1 (0%)	47	58
2	F	434/445 (98%)	419 (96%)	15 (4%)	0	100	100
2	H	434/445 (98%)	415 (96%)	17 (4%)	2 (0%)	29	35
2	J	434/445 (98%)	418 (96%)	16 (4%)	0	100	100
2	L	434/445 (98%)	413 (95%)	21 (5%)	0	100	100
2	N	434/445 (98%)	411 (95%)	23 (5%)	0	100	100
2	P	434/445 (98%)	413 (95%)	20 (5%)	1 (0%)	47	58
All	All	7176/7944 (90%)	6861 (96%)	303 (4%)	12 (0%)	47	58

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	244	ALA
1	M	244	ALA
2	D	645	SER
1	A	244	ALA
2	H	645	SER

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 X-ray entries followed by that with respect to entries of similar resolution.

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	402/469 (86%)	395 (98%)	7 (2%)	60	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	402/469 (86%)	395 (98%)	7 (2%)	60	76
1	E	402/469 (86%)	396 (98%)	6 (2%)	65	79
1	G	402/469 (86%)	393 (98%)	9 (2%)	52	69
1	I	402/469 (86%)	397 (99%)	5 (1%)	71	84
1	K	402/469 (86%)	398 (99%)	4 (1%)	76	87
1	M	402/469 (86%)	392 (98%)	10 (2%)	47	65
1	O	402/469 (86%)	394 (98%)	8 (2%)	55	72
2	B	362/373 (97%)	355 (98%)	7 (2%)	57	73
2	D	362/373 (97%)	352 (97%)	10 (3%)	43	60
2	F	362/373 (97%)	349 (96%)	13 (4%)	35	49
2	H	362/373 (97%)	352 (97%)	10 (3%)	43	60
2	J	362/373 (97%)	349 (96%)	13 (4%)	35	49
2	L	362/373 (97%)	352 (97%)	10 (3%)	43	60
2	N	362/373 (97%)	354 (98%)	8 (2%)	52	69
2	P	362/373 (97%)	350 (97%)	12 (3%)	38	53
All	All	6112/6736 (91%)	5973 (98%)	139 (2%)	50	67

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	810	GLN
1	O	50	LYS
2	P	639	TRP
2	F	943	THR
2	F	902	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	946	ASN
1	O	234	ASN
2	J	723	ASN
1	O	171	GLN
2	P	759	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 ⓘ

72 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	$\# Z > 2$
3	GLC	Q	1	3	12,12,12	0.48	0	17,17,17	0.75	0
3	GLC	Q	2	3	11,11,12	0.29	0	15,15,17	0.72	0
4	NAG	R	1	1,4	14,14,15	0.36	0	17,19,21	0.62	0
4	NAG	R	2	4	14,14,15	0.30	0	17,19,21	0.89	2 (11%)
3	GLC	S	1	3	12,12,12	0.53	0	17,17,17	0.63	0
3	GLC	S	2	3	11,11,12	0.29	0	15,15,17	0.62	0
5	NAG	T	1	5,2	14,14,15	0.49	0	17,19,21	1.04	1 (5%)
5	NAG	T	2	5	14,14,15	0.38	0	17,19,21	0.80	0
5	BMA	T	3	5	11,11,12	0.39	0	15,15,17	0.88	0
3	GLC	U	1	3	12,12,12	0.54	0	17,17,17	0.67	0
3	GLC	U	2	3	11,11,12	0.29	0	15,15,17	0.68	0
4	NAG	V	1	1,4	14,14,15	0.41	0	17,19,21	0.97	0
4	NAG	V	2	4	14,14,15	0.48	0	17,19,21	1.19	2 (11%)
3	GLC	W	1	3	12,12,12	0.49	0	17,17,17	0.76	1 (5%)
3	GLC	W	2	3	11,11,12	0.36	0	15,15,17	1.08	1 (6%)
5	NAG	X	1	5,2	14,14,15	0.58	0	17,19,21	1.15	2 (11%)
5	NAG	X	2	5	14,14,15	0.42	0	17,19,21	1.27	2 (11%)
5	BMA	X	3	5	11,11,12	0.41	0	15,15,17	1.42	2 (13%)
3	GLC	Y	1	3	12,12,12	0.56	0	17,17,17	0.73	0
3	GLC	Y	2	3	11,11,12	0.27	0	15,15,17	0.76	0
4	NAG	Z	1	1,4	14,14,15	0.38	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	Z	2	4	14,14,15	0.42	0	17,19,21	0.89	0
3	GLC	a	1	3	12,12,12	0.45	0	17,17,17	0.56	0
3	GLC	a	2	3	11,11,12	0.29	0	15,15,17	0.62	0
5	NAG	b	1	5,2	14,14,15	0.55	0	17,19,21	0.91	1 (5%)
5	NAG	b	2	5	14,14,15	0.48	0	17,19,21	1.82	3 (17%)
5	BMA	b	3	5	11,11,12	0.43	0	15,15,17	0.99	1 (6%)
3	GLC	c	1	3	12,12,12	0.44	0	17,17,17	0.63	0
3	GLC	c	2	3	11,11,12	0.29	0	15,15,17	0.52	0
4	NAG	d	1	1,4	14,14,15	0.39	0	17,19,21	0.75	1 (5%)
4	NAG	d	2	4	14,14,15	0.42	0	17,19,21	0.90	0
3	GLC	e	1	3	12,12,12	0.50	0	17,17,17	0.73	0
3	GLC	e	2	3	11,11,12	0.37	0	15,15,17	0.51	0
5	NAG	f	1	5,2	14,14,15	0.59	0	17,19,21	0.87	0
5	NAG	f	2	5	14,14,15	0.50	0	17,19,21	1.67	4 (23%)
5	BMA	f	3	5	11,11,12	0.41	0	15,15,17	0.96	1 (6%)
3	GLC	g	1	3	12,12,12	0.52	0	17,17,17	0.56	0
3	GLC	g	2	3	11,11,12	0.26	0	15,15,17	0.80	0
4	NAG	h	1	1,4	14,14,15	0.49	0	17,19,21	0.94	1 (5%)
4	NAG	h	2	4	14,14,15	0.43	0	17,19,21	1.08	1 (5%)
3	GLC	i	1	3	12,12,12	0.59	0	17,17,17	1.23	2 (11%)
3	GLC	i	2	3	11,11,12	0.31	0	15,15,17	0.87	0
5	NAG	j	1	5,2	14,14,15	0.42	0	17,19,21	0.74	0
5	NAG	j	2	5	14,14,15	0.46	0	17,19,21	1.20	2 (11%)
5	BMA	j	3	5	11,11,12	0.38	0	15,15,17	1.03	0
3	GLC	k	1	3	12,12,12	0.45	0	17,17,17	0.86	0
3	GLC	k	2	3	11,11,12	0.31	0	15,15,17	0.70	0
4	NAG	l	1	1,4	14,14,15	0.40	0	17,19,21	0.76	0
4	NAG	l	2	4	14,14,15	0.34	0	17,19,21	1.10	1 (5%)
3	GLC	m	1	3	12,12,12	0.50	0	17,17,17	0.74	0
3	GLC	m	2	3	11,11,12	0.32	0	15,15,17	0.55	0
5	NAG	n	1	5,2	14,14,15	0.45	0	17,19,21	1.04	1 (5%)
5	NAG	n	2	5	14,14,15	0.36	0	17,19,21	1.18	2 (11%)
5	BMA	n	3	5	11,11,12	0.42	0	15,15,17	1.03	1 (6%)
3	GLC	o	1	3	12,12,12	0.57	0	17,17,17	0.75	0
3	GLC	o	2	3	11,11,12	0.33	0	15,15,17	0.86	0
4	NAG	p	1	1,4	14,14,15	0.41	0	17,19,21	0.83	0
4	NAG	p	2	4	14,14,15	0.33	0	17,19,21	1.14	2 (11%)
3	GLC	q	1	3	12,12,12	0.53	0	17,17,17	0.72	0
3	GLC	q	2	3	11,11,12	0.28	0	15,15,17	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	r	1	5,2	14,14,15	0.42	0	17,19,21	1.56	3 (17%)
5	NAG	r	2	5	14,14,15	0.37	0	17,19,21	1.13	2 (11%)
5	BMA	r	3	5	11,11,12	0.41	0	15,15,17	1.01	0
3	GLC	s	1	3	12,12,12	0.51	0	17,17,17	0.43	0
3	GLC	s	2	3	11,11,12	0.32	0	15,15,17	0.63	0
4	NAG	t	1	1,4	14,14,15	0.36	0	17,19,21	0.90	1 (5%)
4	NAG	t	2	4	14,14,15	0.36	0	17,19,21	1.11	1 (5%)
3	GLC	u	1	3	12,12,12	0.57	0	17,17,17	0.71	0
3	GLC	u	2	3	11,11,12	0.27	0	15,15,17	0.64	0
5	NAG	v	1	5,2	14,14,15	0.47	0	17,19,21	1.05	1 (5%)
5	NAG	v	2	5	14,14,15	0.40	0	17,19,21	1.01	0
5	BMA	v	3	5	11,11,12	0.39	0	15,15,17	0.92	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
3	GLC	Q	1	3	-	0/2/22/22	0/1/1/1
3	GLC	Q	2	3	-	0/2/19/22	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
3	GLC	S	1	3	-	0/2/22/22	0/1/1/1
3	GLC	S	2	3	-	0/2/19/22	0/1/1/1
5	NAG	T	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
3	GLC	U	1	3	-	0/2/22/22	0/1/1/1
3	GLC	U	2	3	-	0/2/19/22	0/1/1/1
4	NAG	V	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
3	GLC	W	1	3	-	2/2/22/22	0/1/1/1
3	GLC	W	2	3	-	2/2/19/22	0/1/1/1
5	NAG	X	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	1/6/23/26	0/1/1/1
5	BMA	X	3	5	-	2/2/19/22	0/1/1/1
3	GLC	Y	1	3	-	0/2/22/22	0/1/1/1
3	GLC	Y	2	3	-	0/2/19/22	0/1/1/1
4	NAG	Z	1	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1
3	GLC	a	1	3	-	0/2/22/22	0/1/1/1
3	GLC	a	2	3	-	0/2/19/22	0/1/1/1
5	NAG	b	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	1/6/23/26	0/1/1/1
5	BMA	b	3	5	-	2/2/19/22	0/1/1/1
3	GLC	c	1	3	-	0/2/22/22	0/1/1/1
3	GLC	c	2	3	-	0/2/19/22	0/1/1/1
4	NAG	d	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1
3	GLC	e	1	3	-	1/2/22/22	0/1/1/1
3	GLC	e	2	3	-	0/2/19/22	0/1/1/1
5	NAG	f	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	f	2	5	-	0/6/23/26	0/1/1/1
5	BMA	f	3	5	-	2/2/19/22	0/1/1/1
3	GLC	g	1	3	-	0/2/22/22	0/1/1/1
3	GLC	g	2	3	-	0/2/19/22	0/1/1/1
4	NAG	h	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	h	2	4	-	0/6/23/26	0/1/1/1
3	GLC	i	1	3	-	0/2/22/22	0/1/1/1
3	GLC	i	2	3	-	0/2/19/22	0/1/1/1
5	NAG	j	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	j	2	5	-	2/6/23/26	0/1/1/1
5	BMA	j	3	5	-	2/2/19/22	0/1/1/1
3	GLC	k	1	3	-	0/2/22/22	0/1/1/1
3	GLC	k	2	3	-	0/2/19/22	0/1/1/1
4	NAG	l	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	l	2	4	-	0/6/23/26	0/1/1/1
3	GLC	m	1	3	-	0/2/22/22	0/1/1/1
3	GLC	m	2	3	-	0/2/19/22	0/1/1/1
5	NAG	n	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	n	2	5	-	2/6/23/26	0/1/1/1
5	BMA	n	3	5	-	2/2/19/22	0/1/1/1
3	GLC	o	1	3	-	0/2/22/22	0/1/1/1
3	GLC	o	2	3	-	0/2/19/22	0/1/1/1
4	NAG	p	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	p	2	4	-	0/6/23/26	0/1/1/1
3	GLC	q	1	3	-	0/2/22/22	0/1/1/1
3	GLC	q	2	3	-	0/2/19/22	0/1/1/1
5	NAG	r	1	5,2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	r	2	5	-	1/6/23/26	0/1/1/1
5	BMA	r	3	5	-	2/2/19/22	0/1/1/1
3	GLC	s	1	3	-	0/2/22/22	0/1/1/1
3	GLC	s	2	3	-	0/2/19/22	0/1/1/1
4	NAG	t	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	t	2	4	-	0/6/23/26	0/1/1/1
3	GLC	u	1	3	-	0/2/22/22	0/1/1/1
3	GLC	u	2	3	-	0/2/19/22	0/1/1/1
5	NAG	v	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	v	2	5	-	2/6/23/26	0/1/1/1
5	BMA	v	3	5	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	2	NAG	C1-O5-C5	5.29	119.36	112.19
5	f	2	NAG	C4-C3-C2	4.06	116.97	111.02
5	r	1	NAG	C2-N2-C7	4.03	128.65	122.90
4	t	2	NAG	C1-O5-C5	3.58	117.05	112.19
4	l	2	NAG	C1-O5-C5	3.42	116.83	112.19

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	r	3	BMA	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
5	b	3	BMA	O5-C5-C6-O6
5	n	3	BMA	O5-C5-C6-O6
3	W	2	GLC	C4-C5-C6-O6

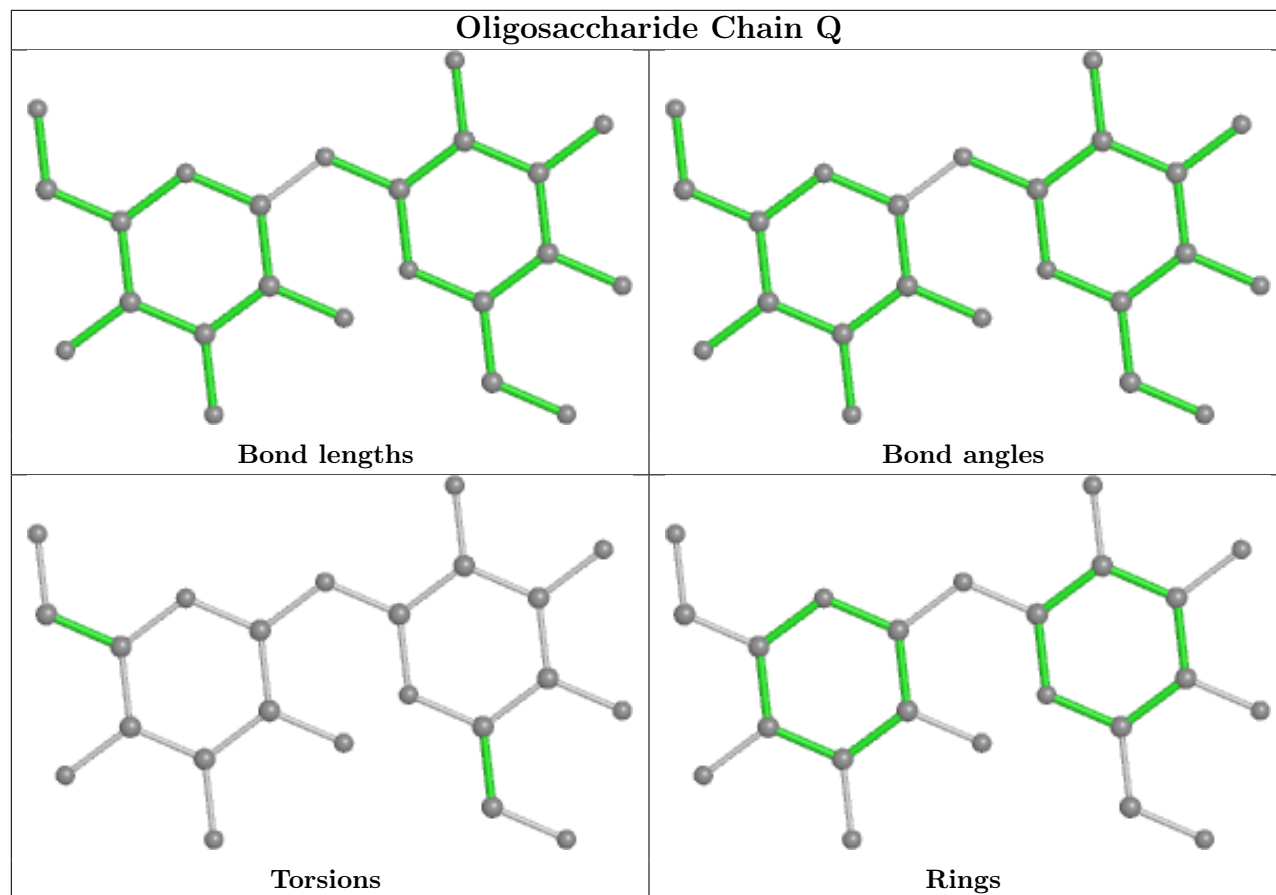
There are no ring outliers.

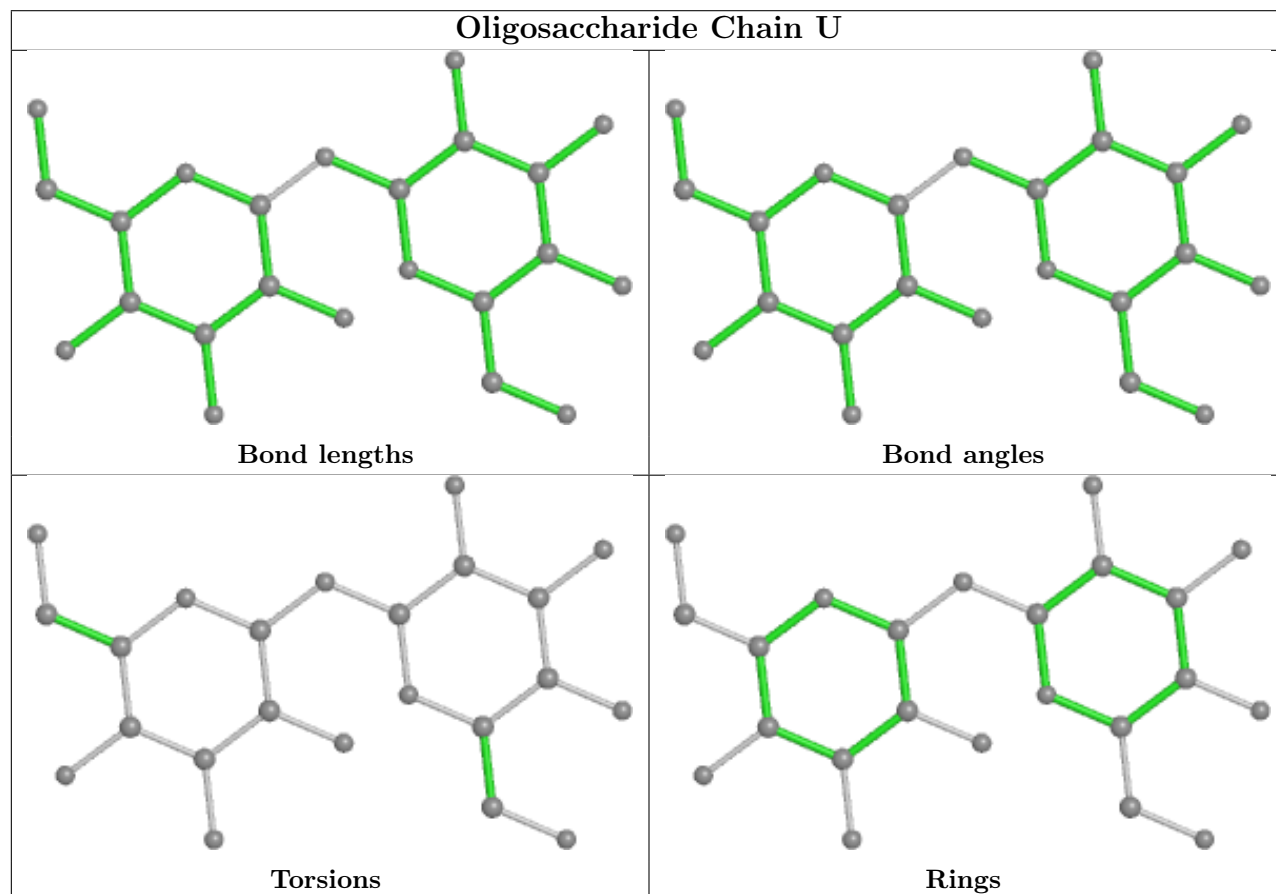
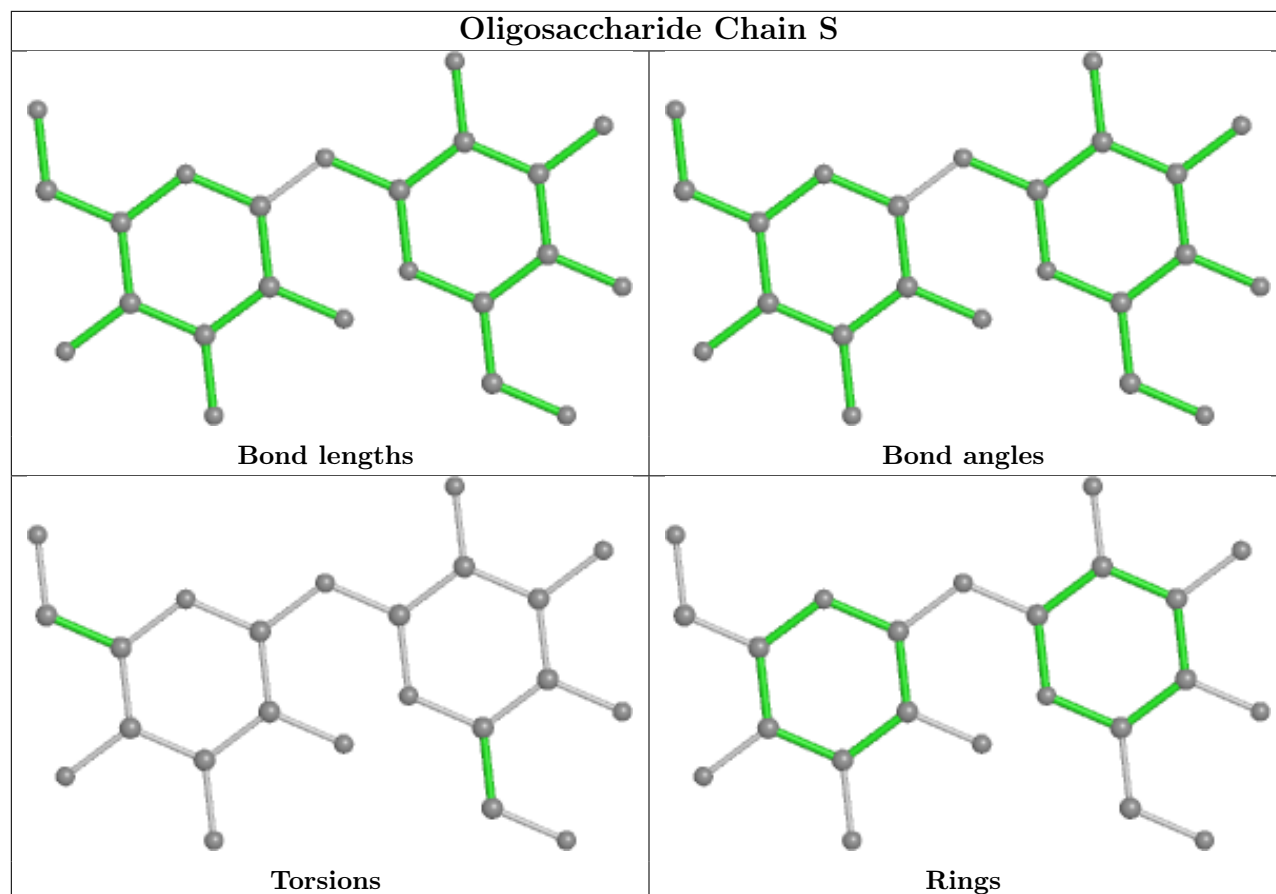
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	2	NAG	1	0
5	T	3	BMA	1	0

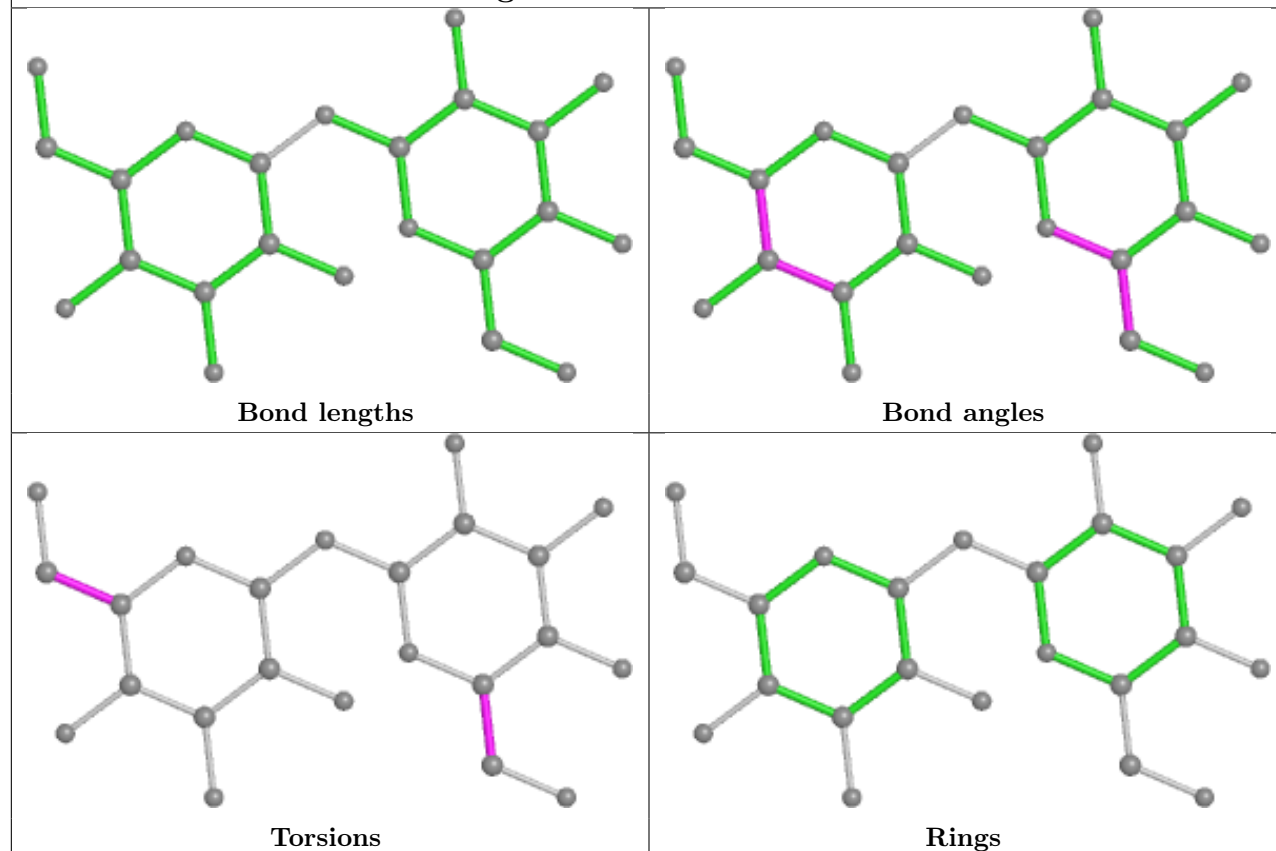
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

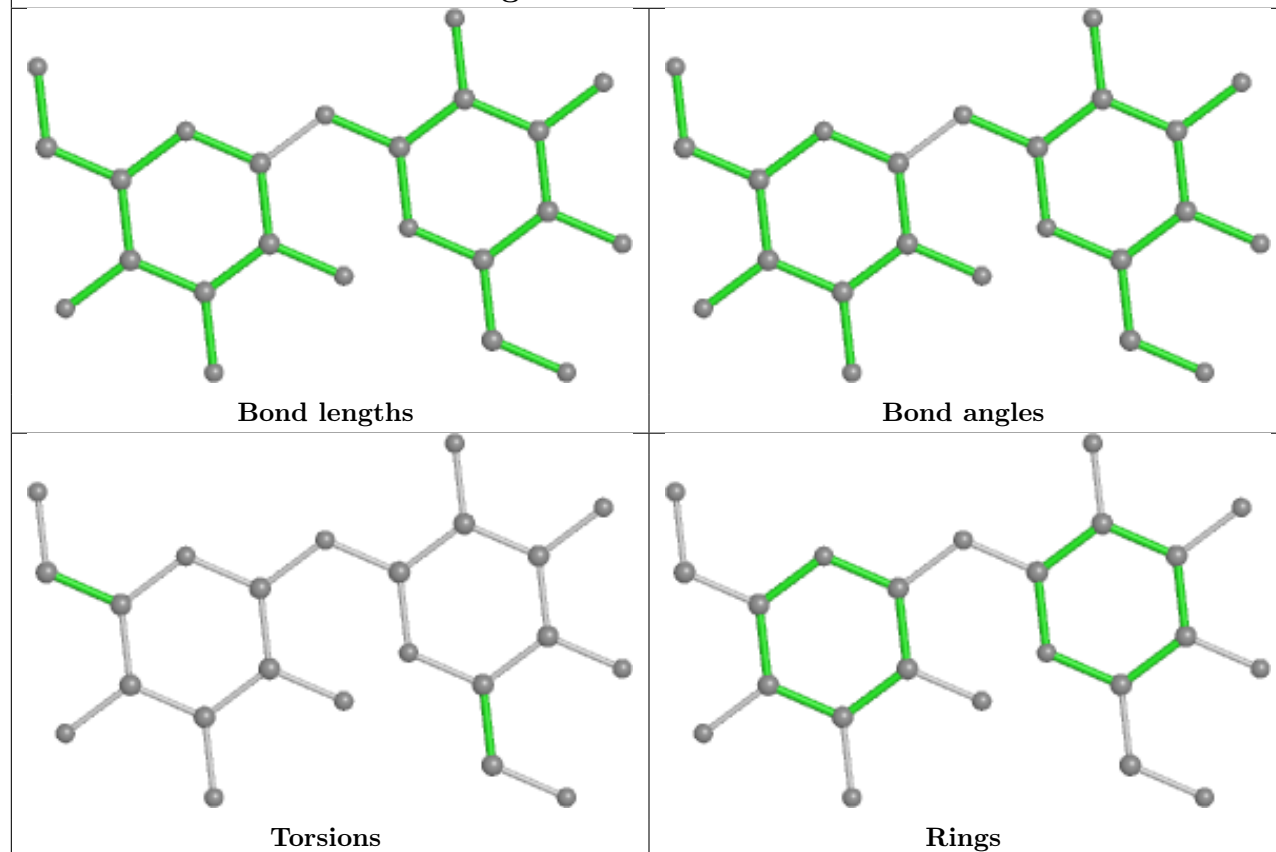


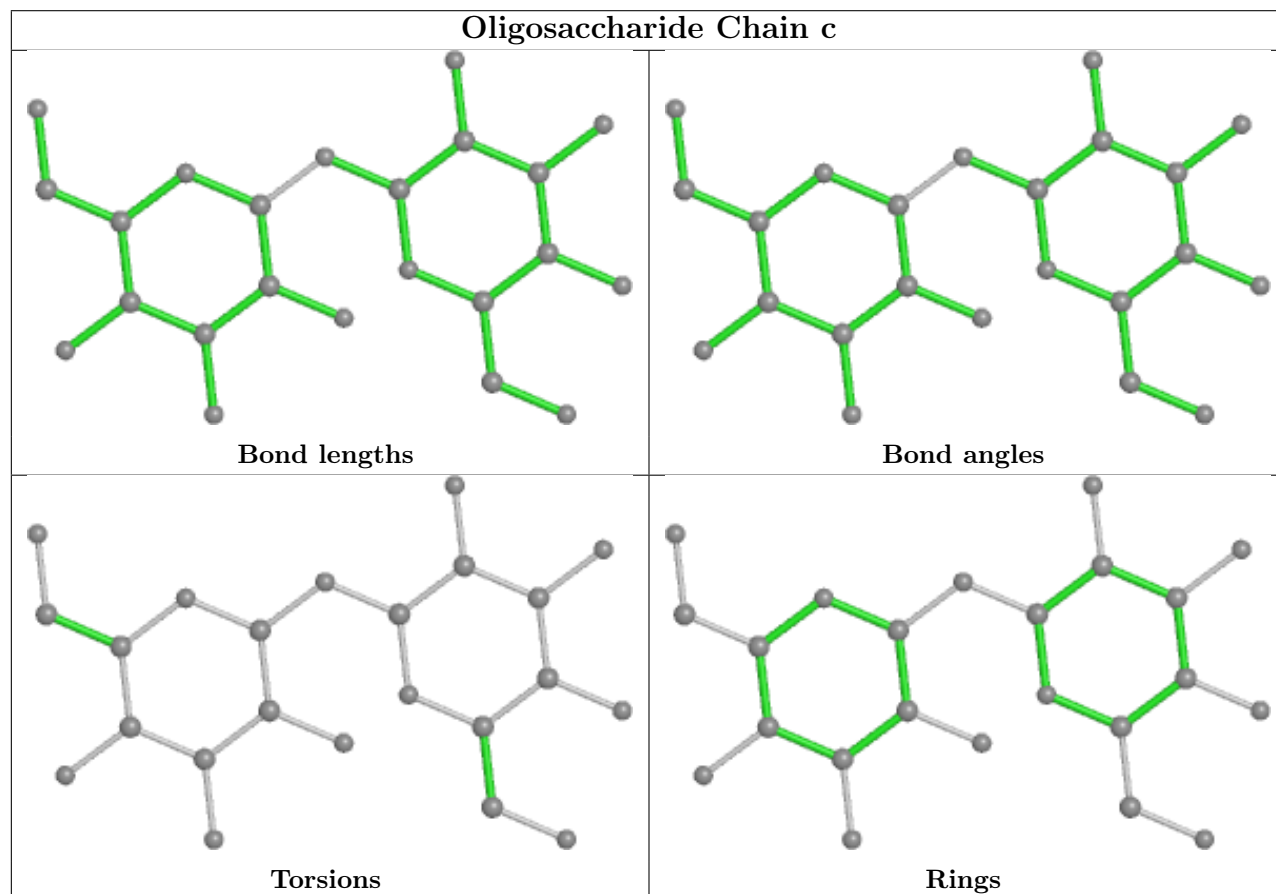
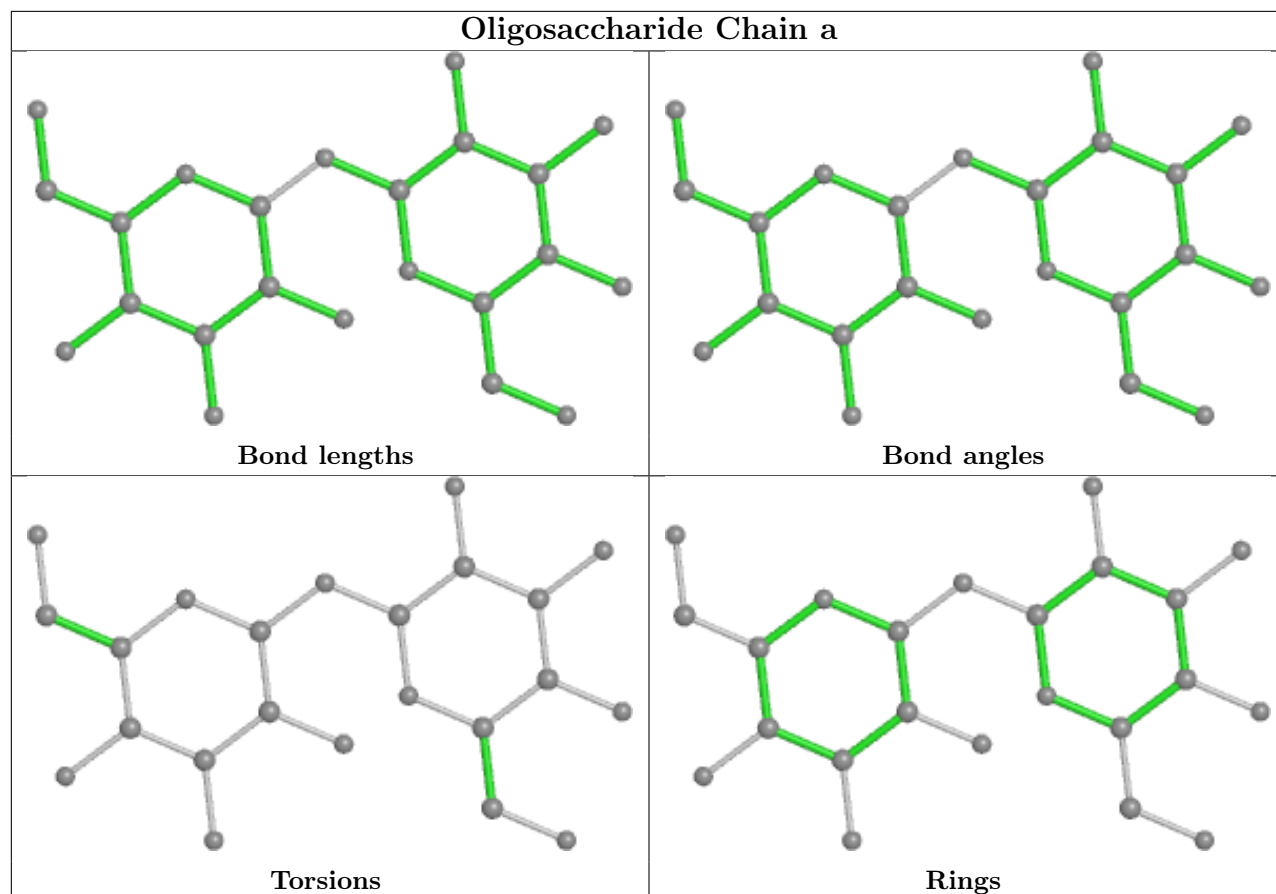


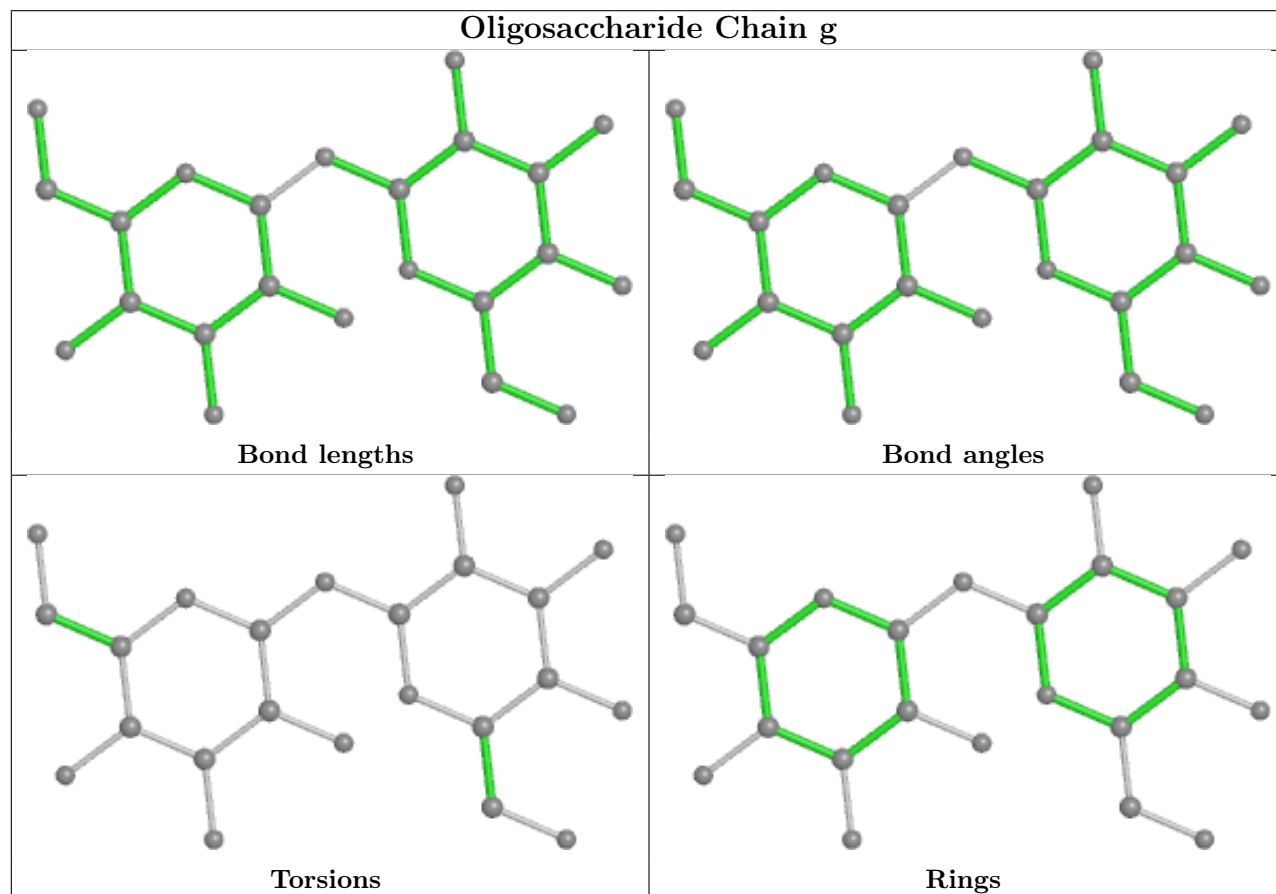
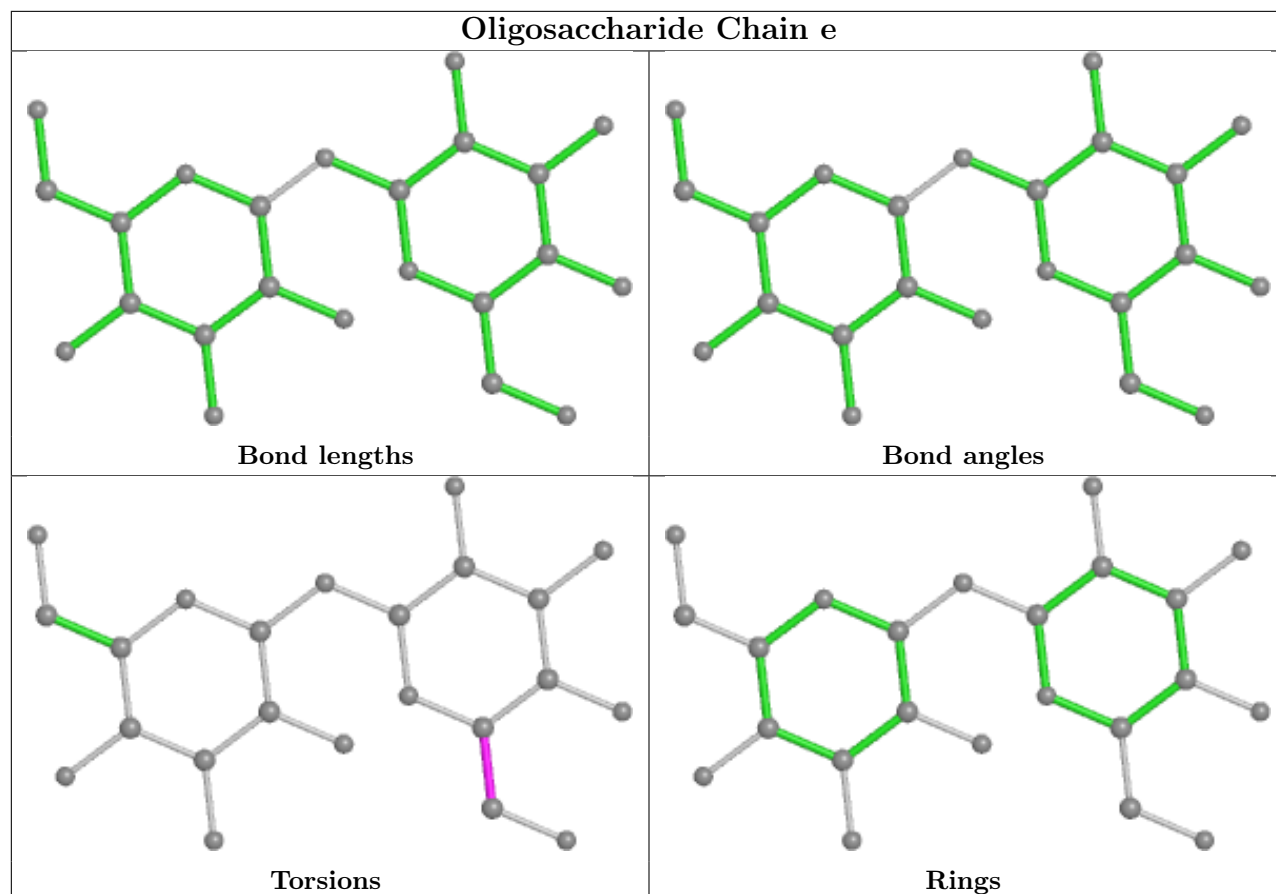
Oligosaccharide Chain W

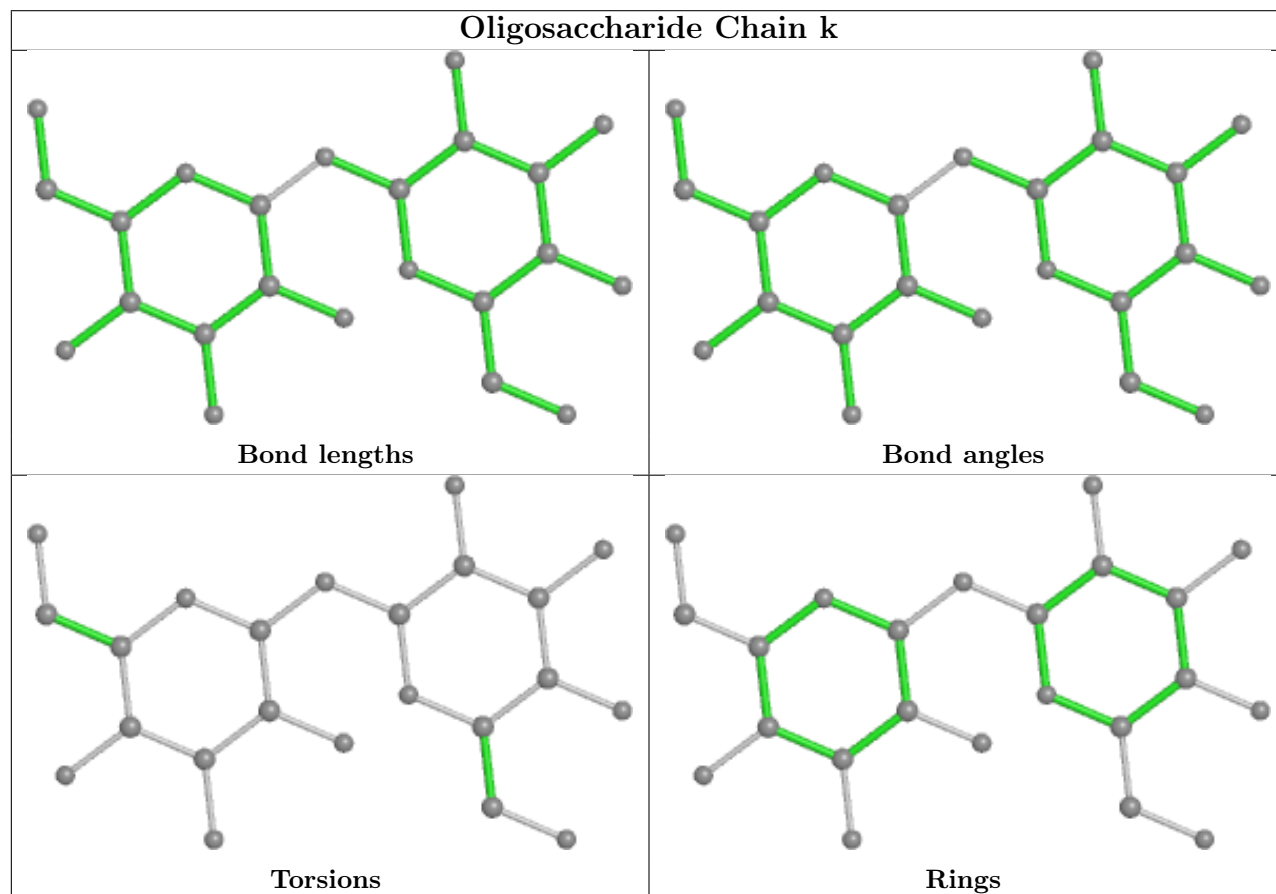
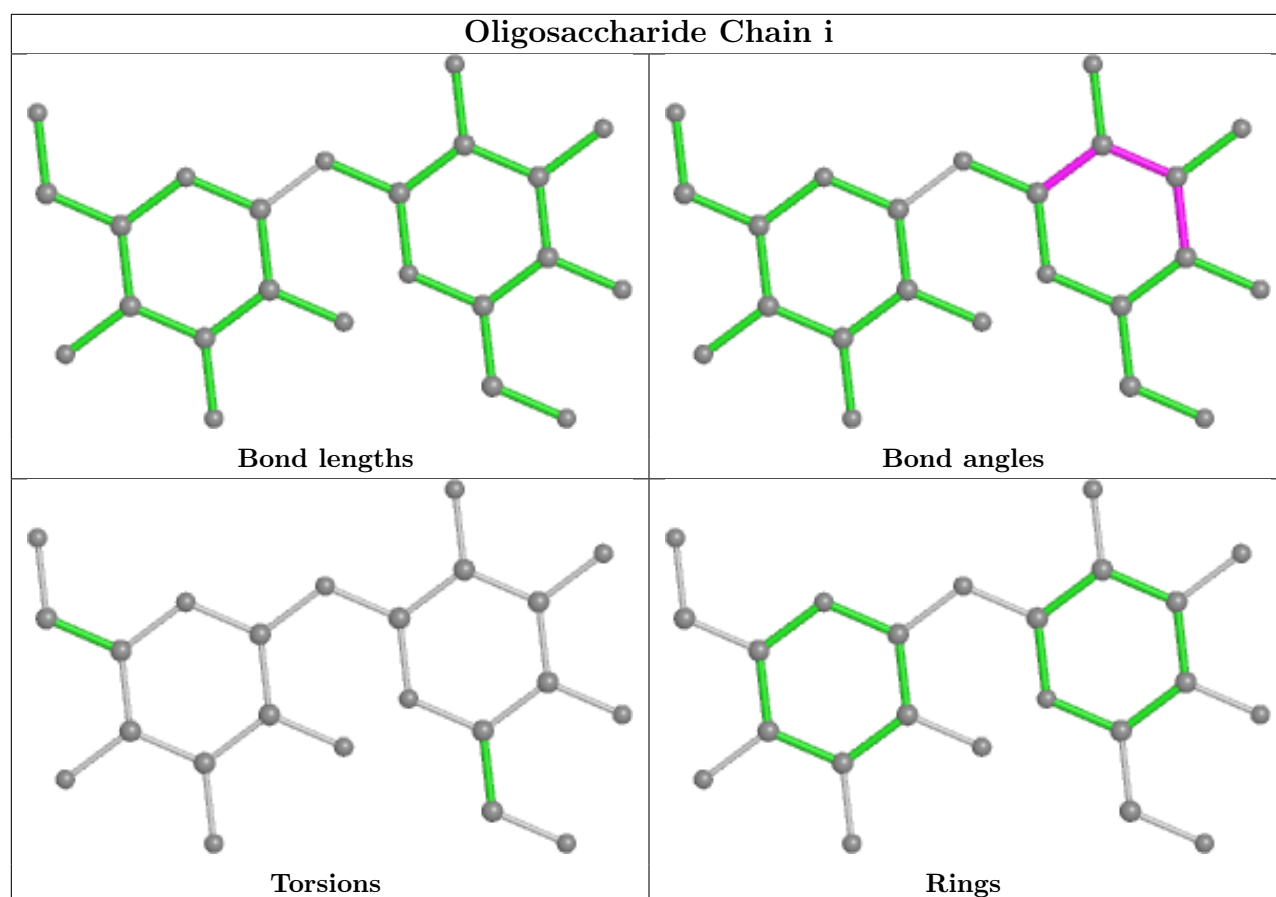


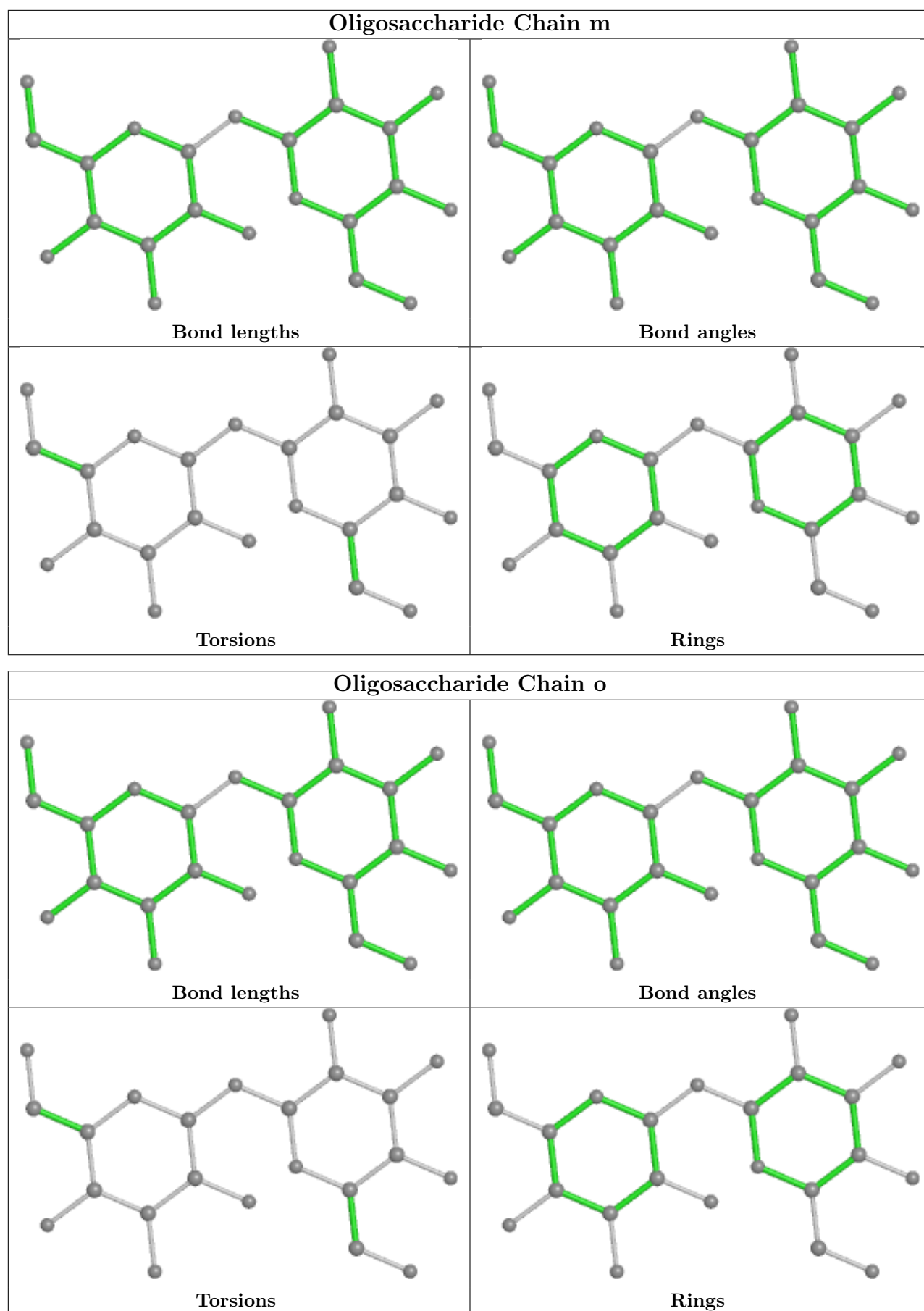
Oligosaccharide Chain Y

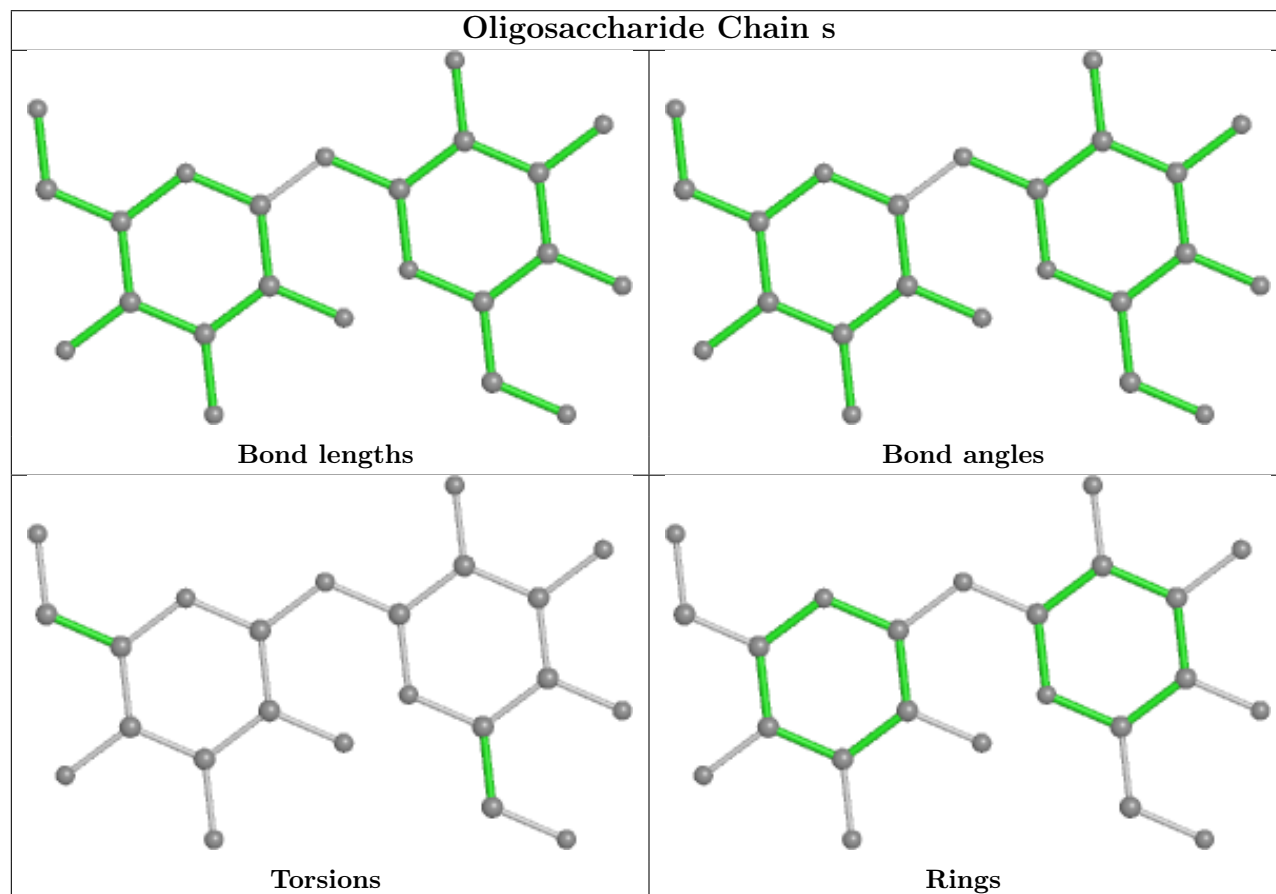
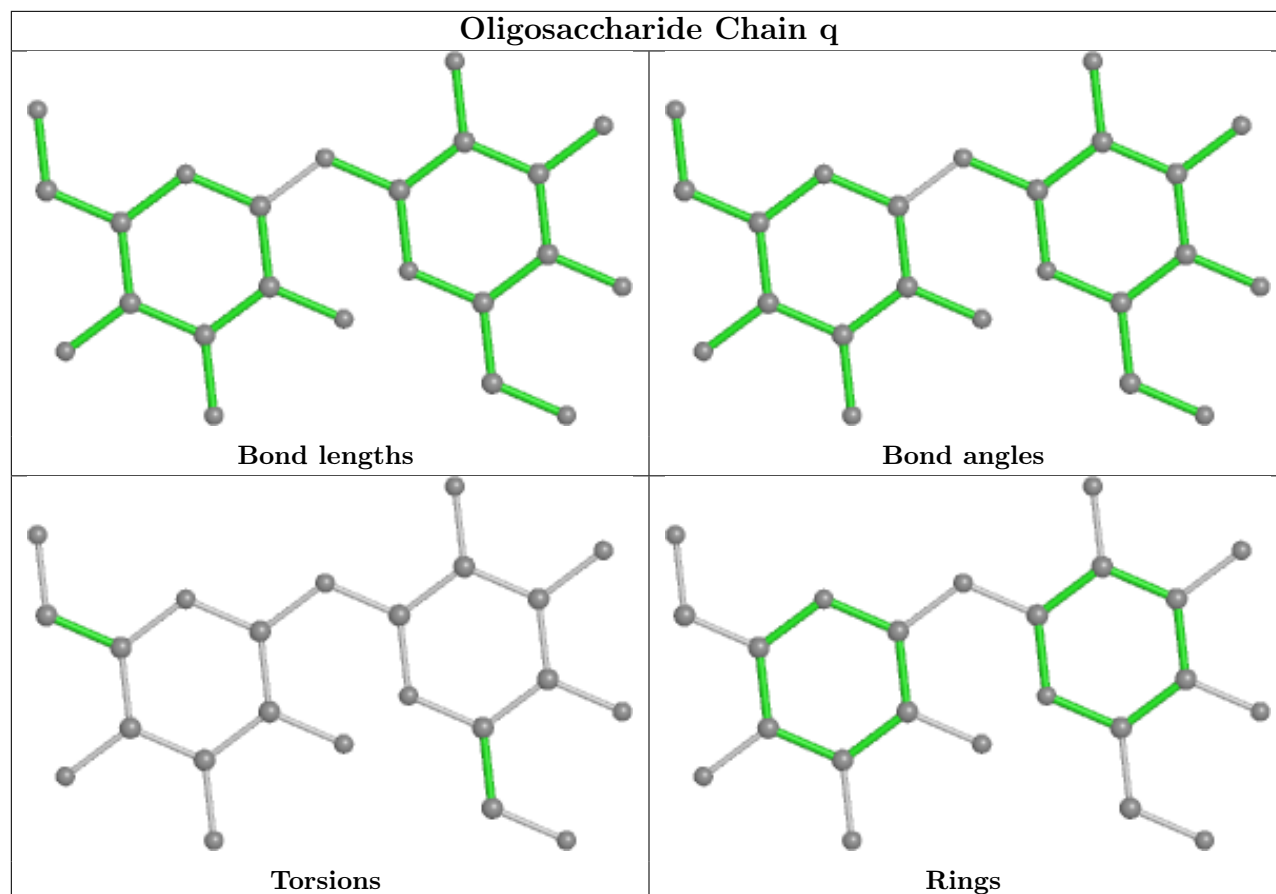


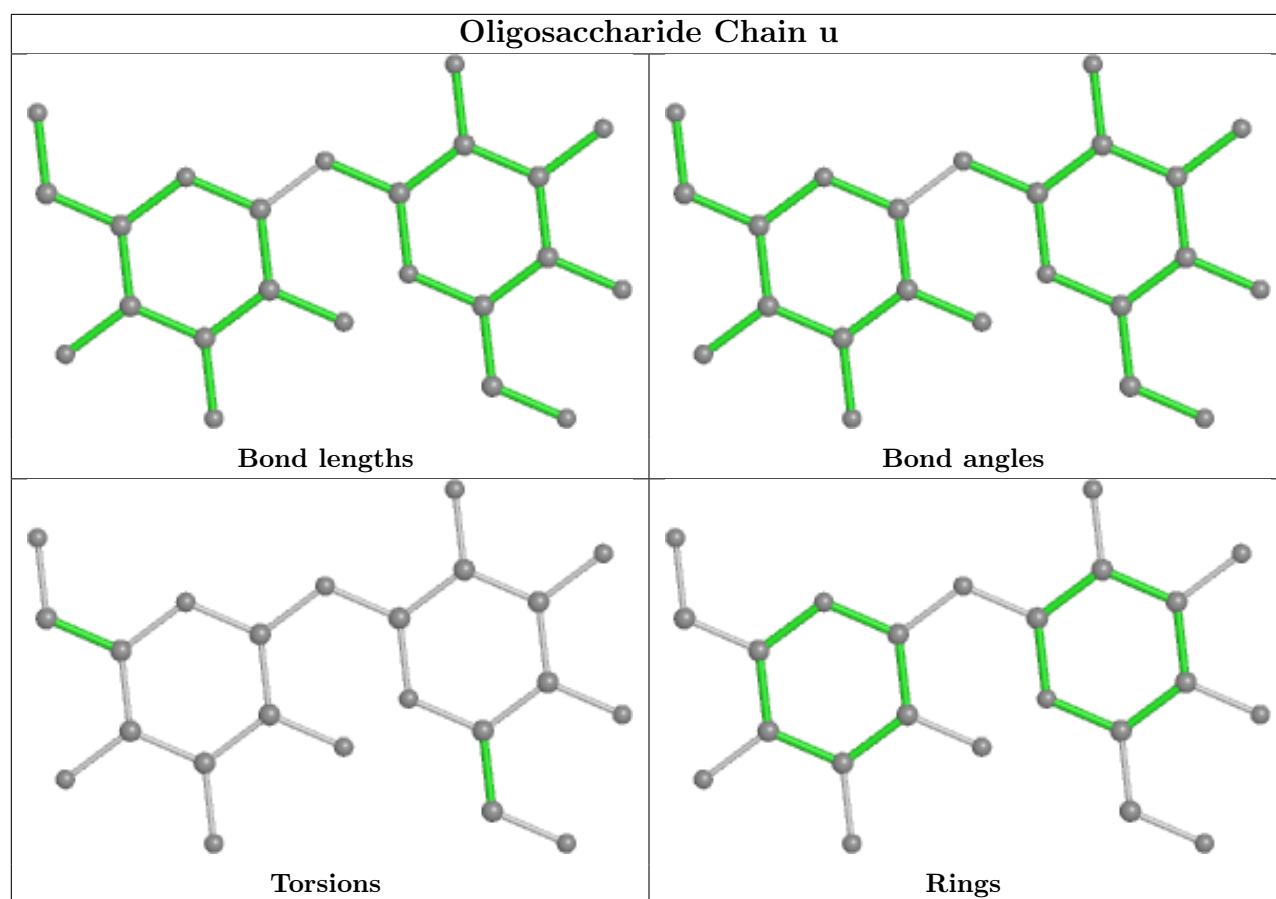


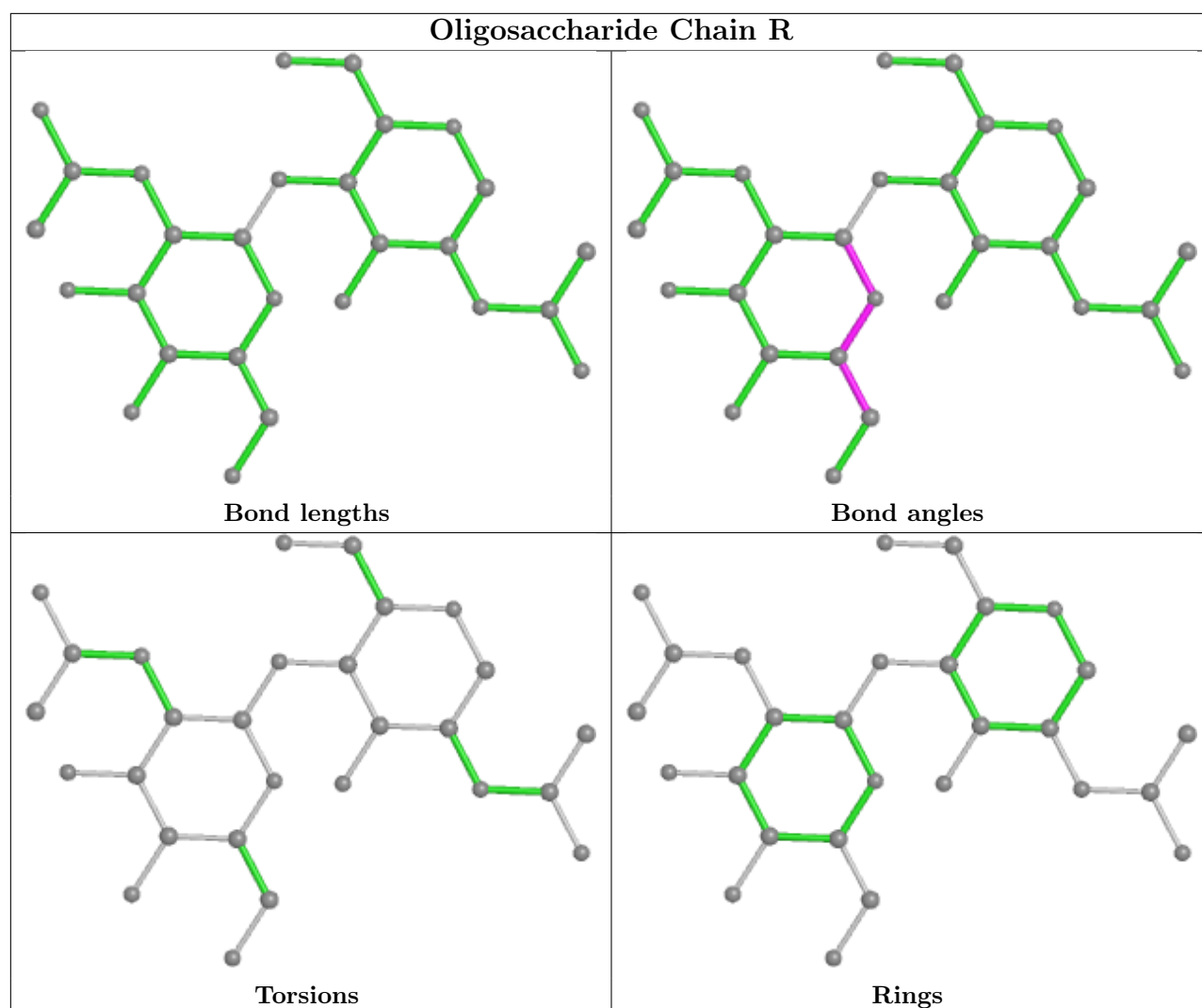


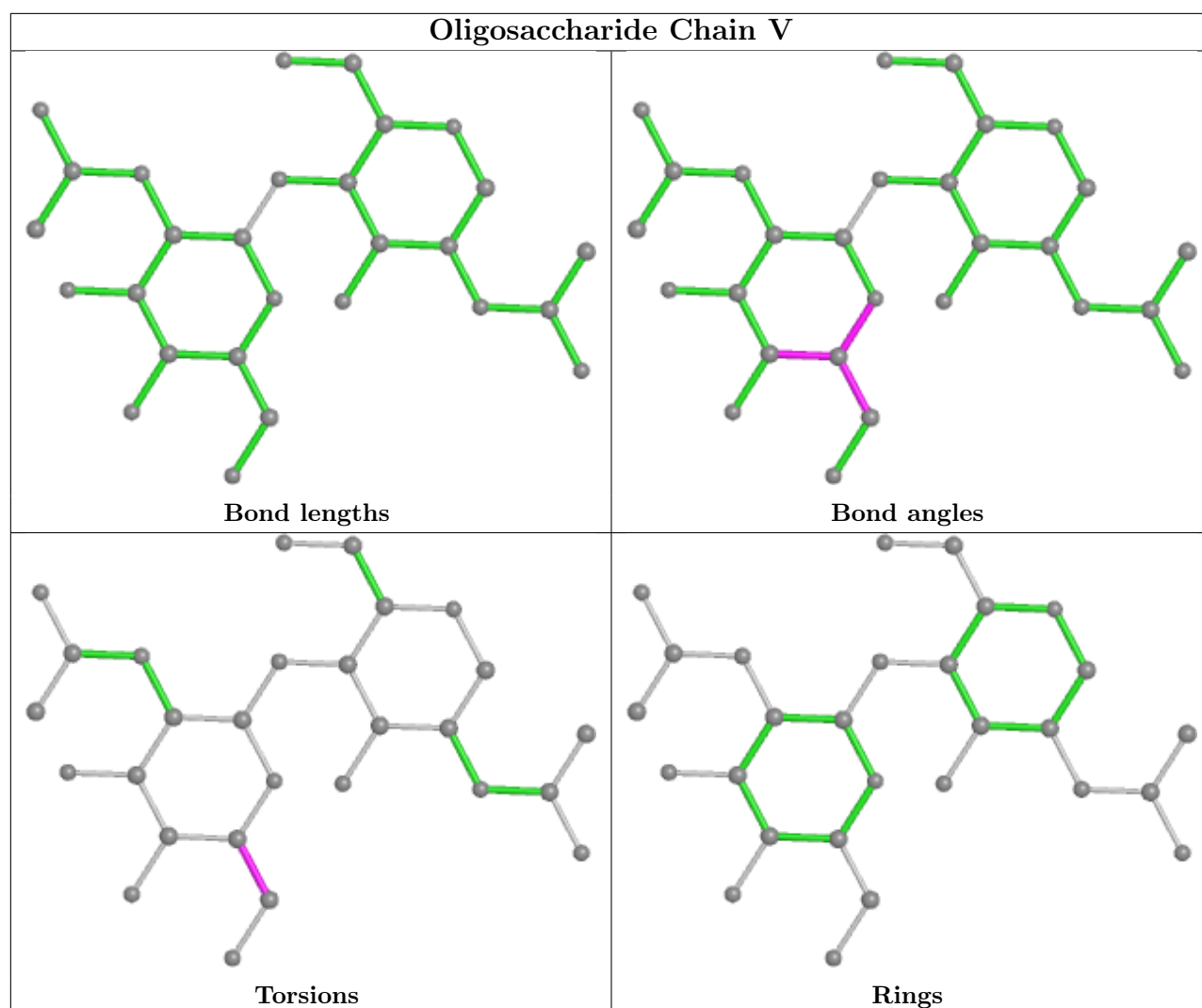


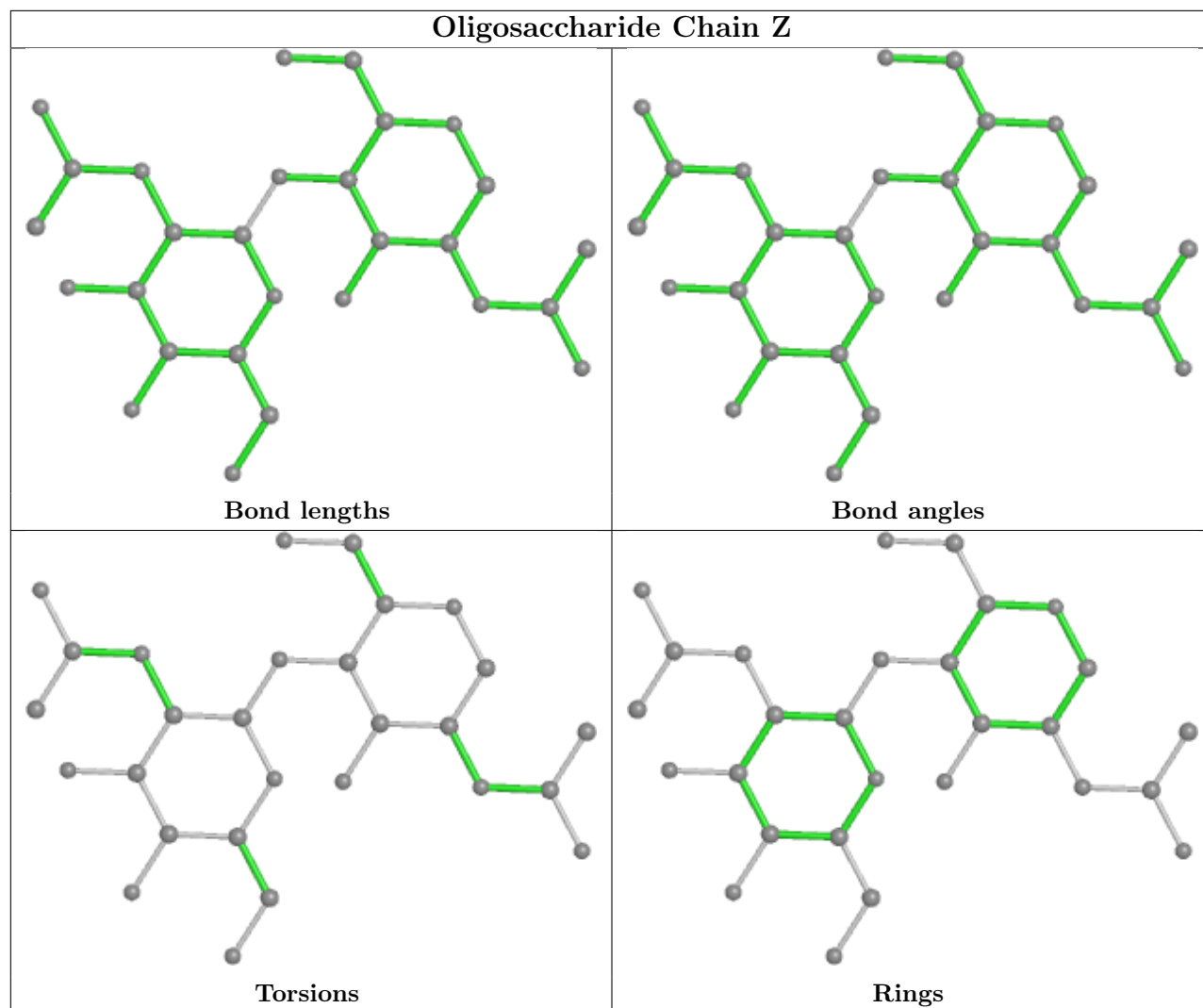


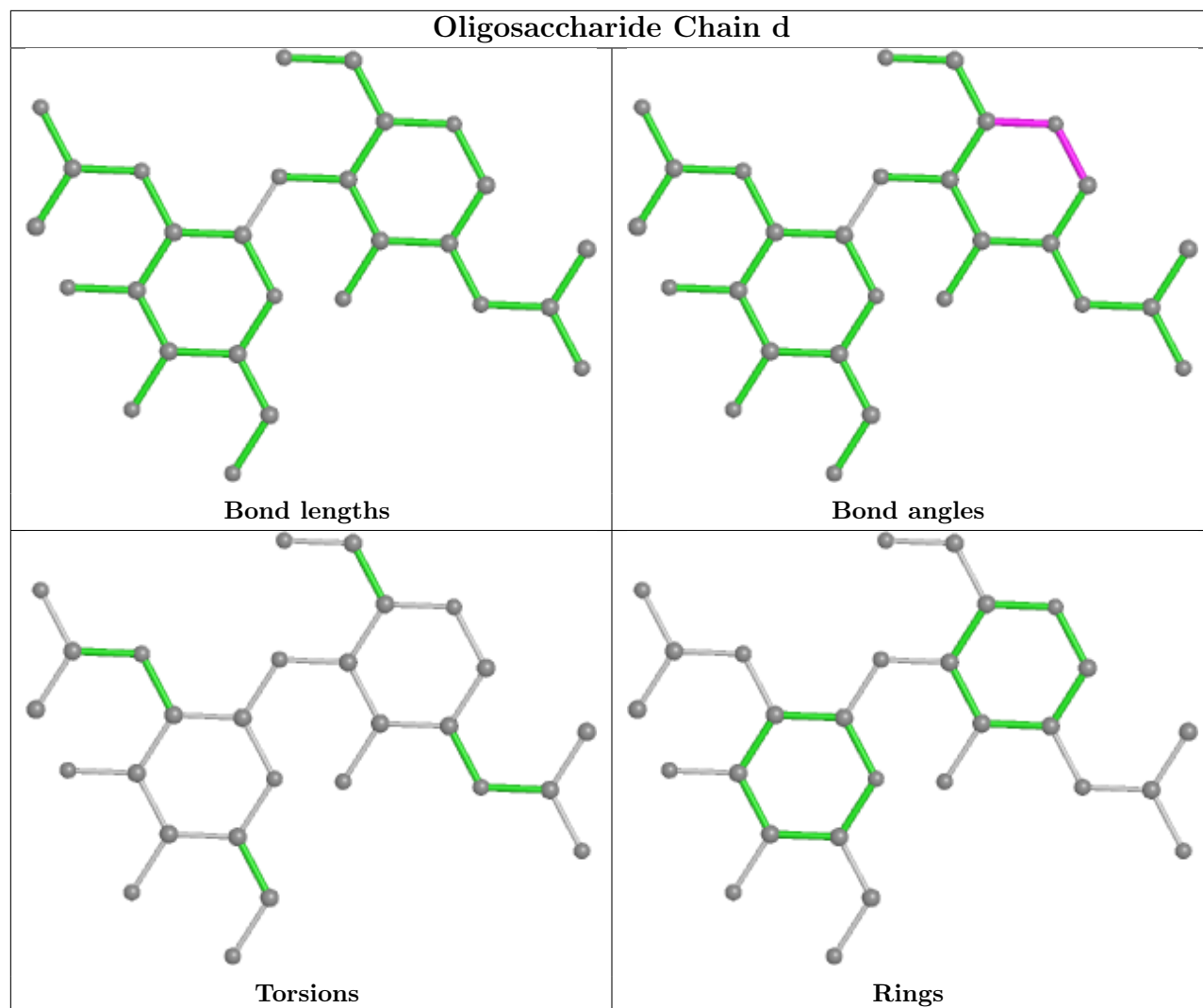


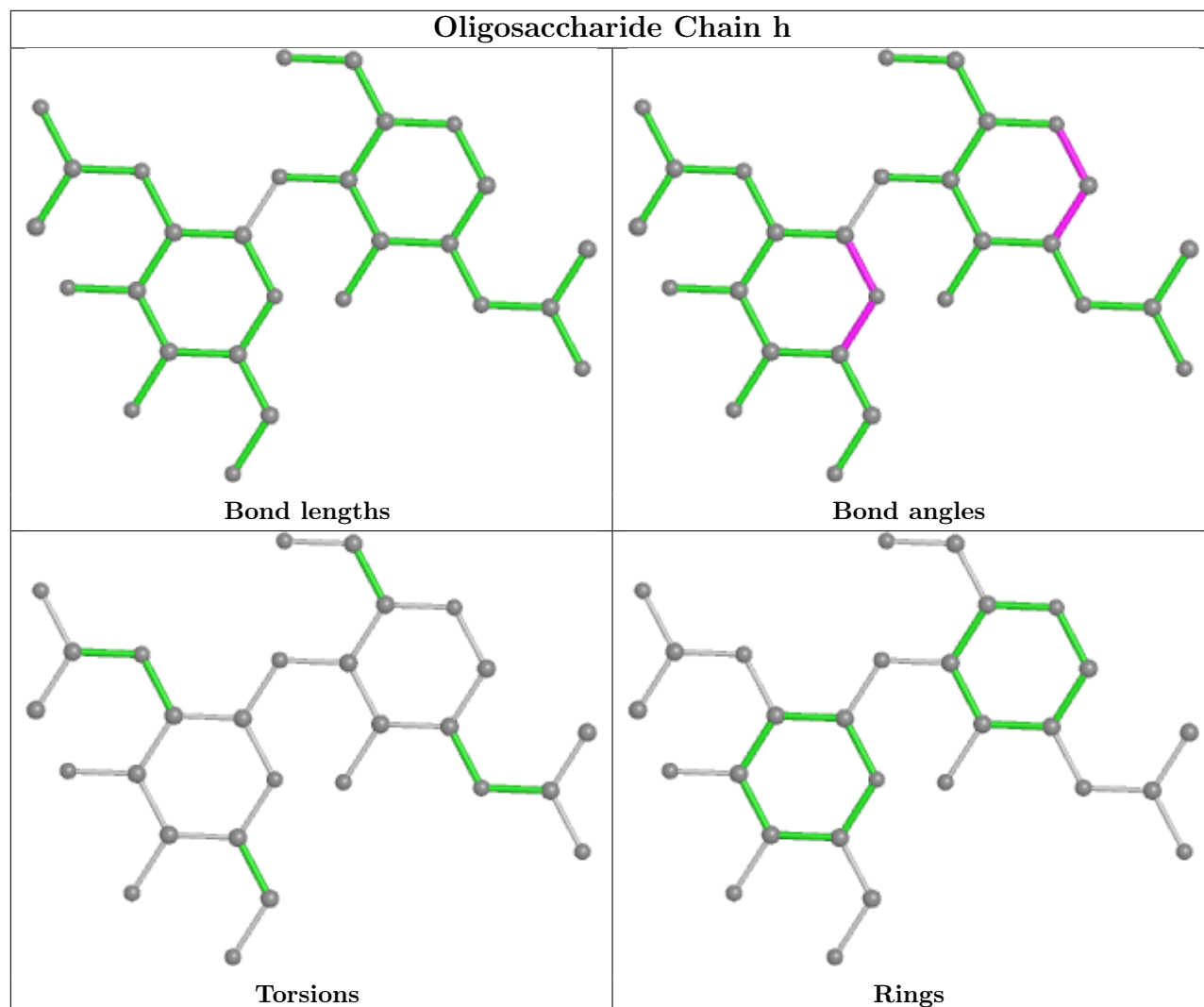


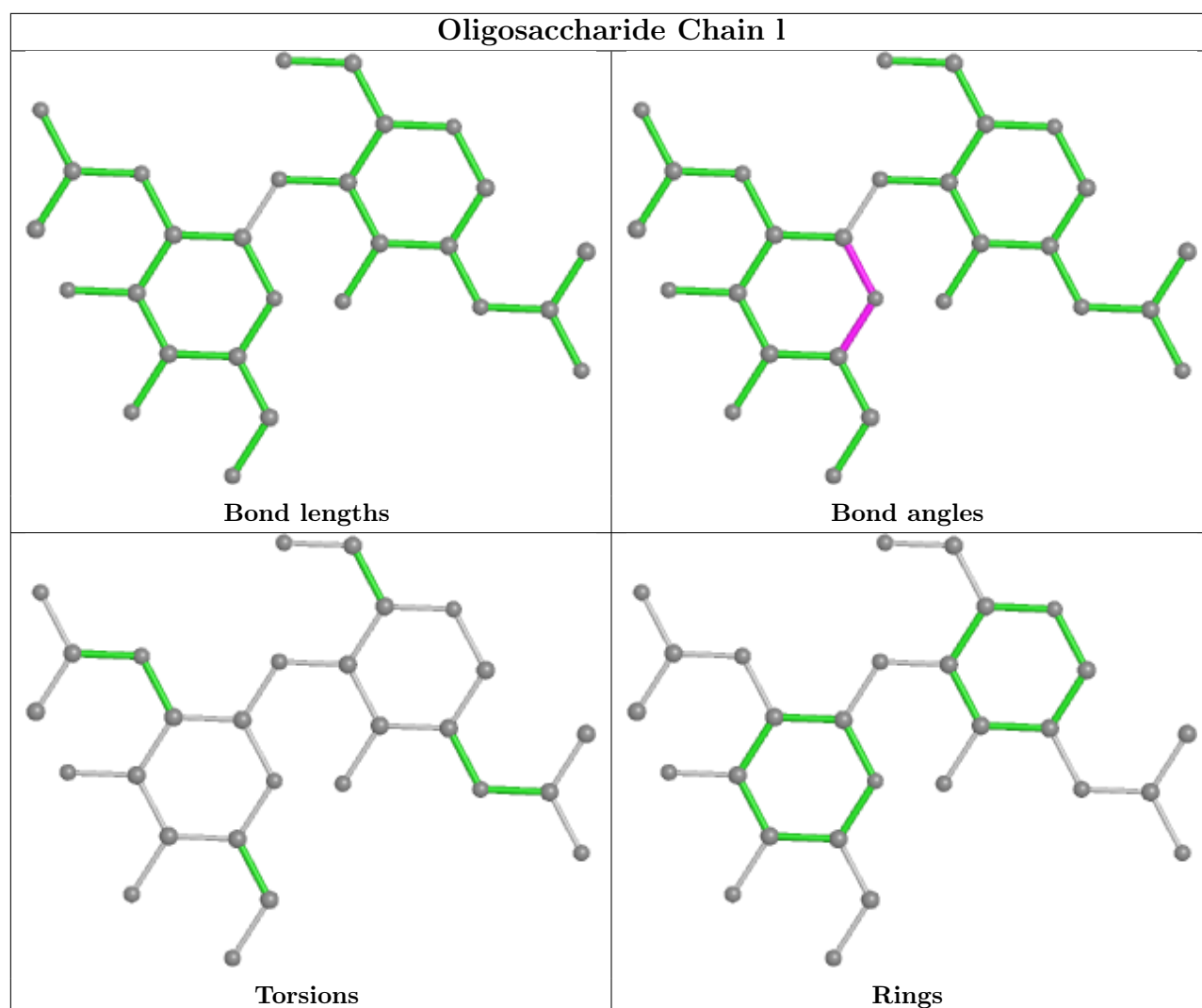


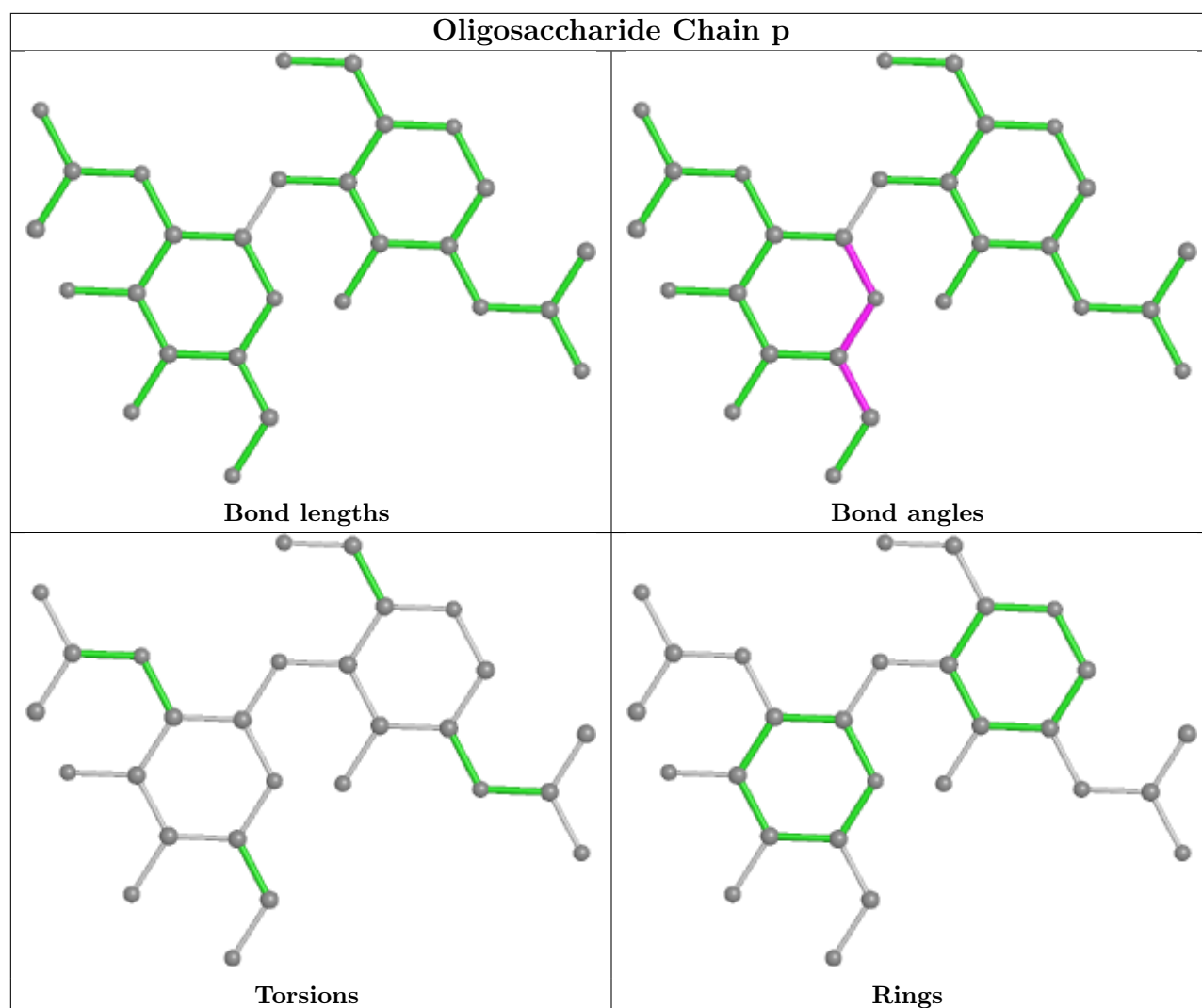


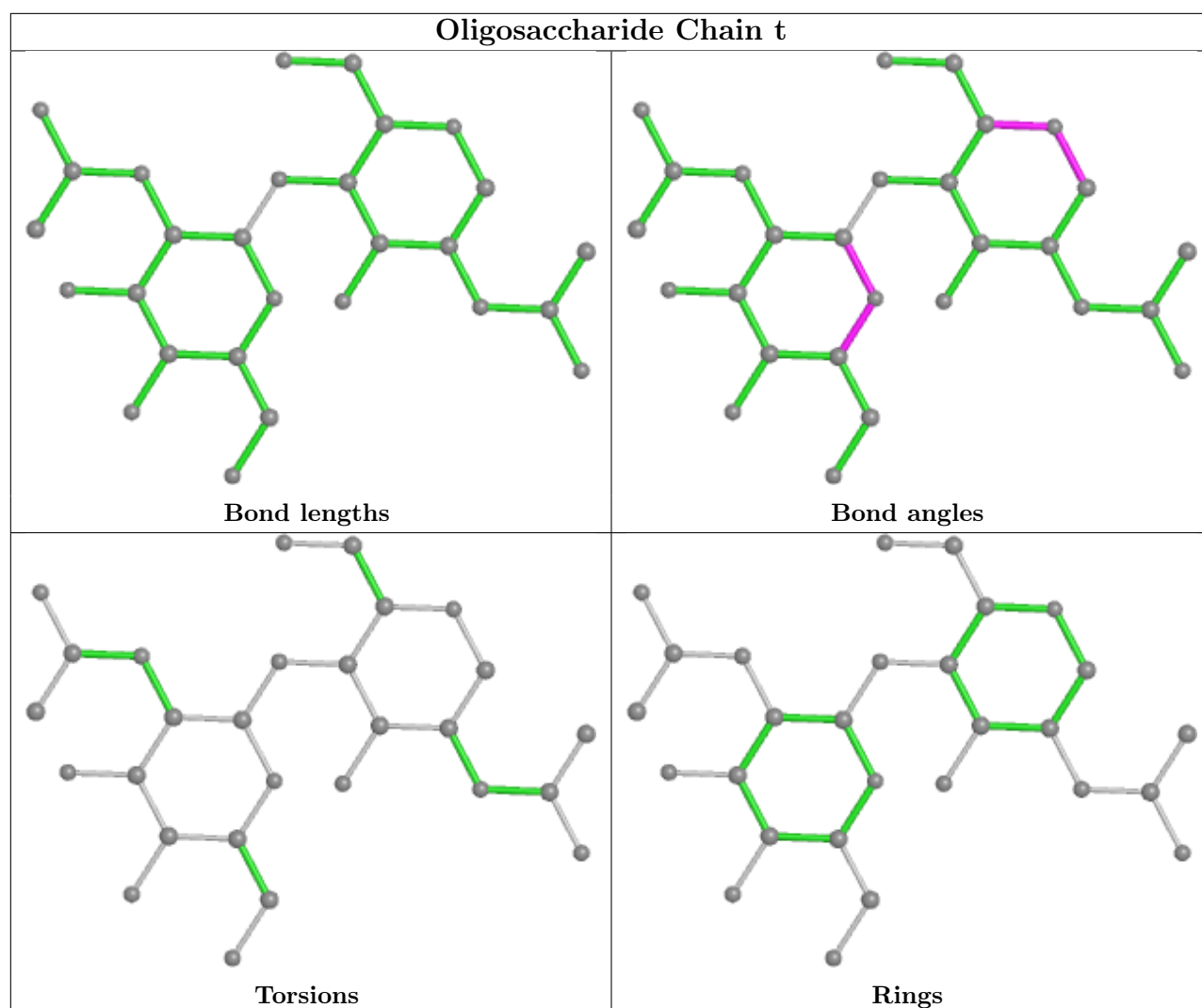


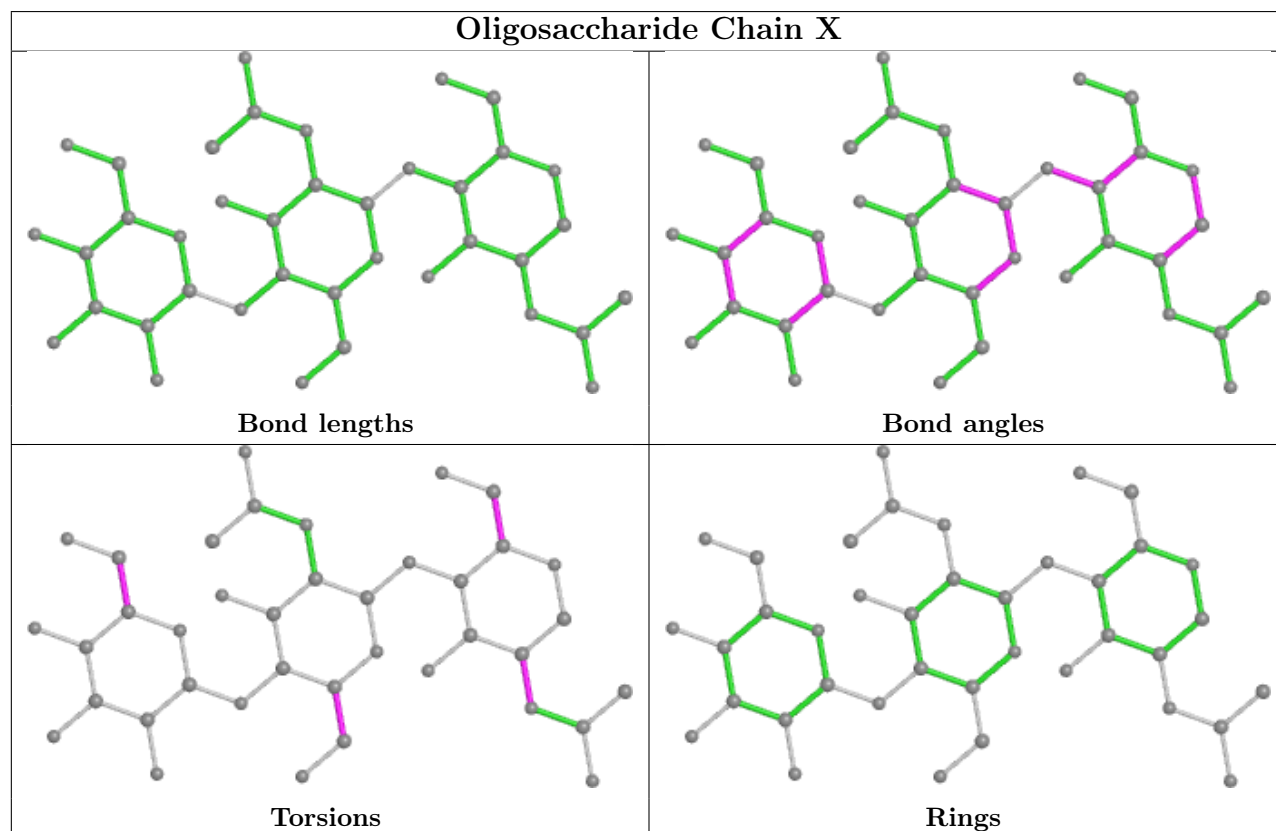
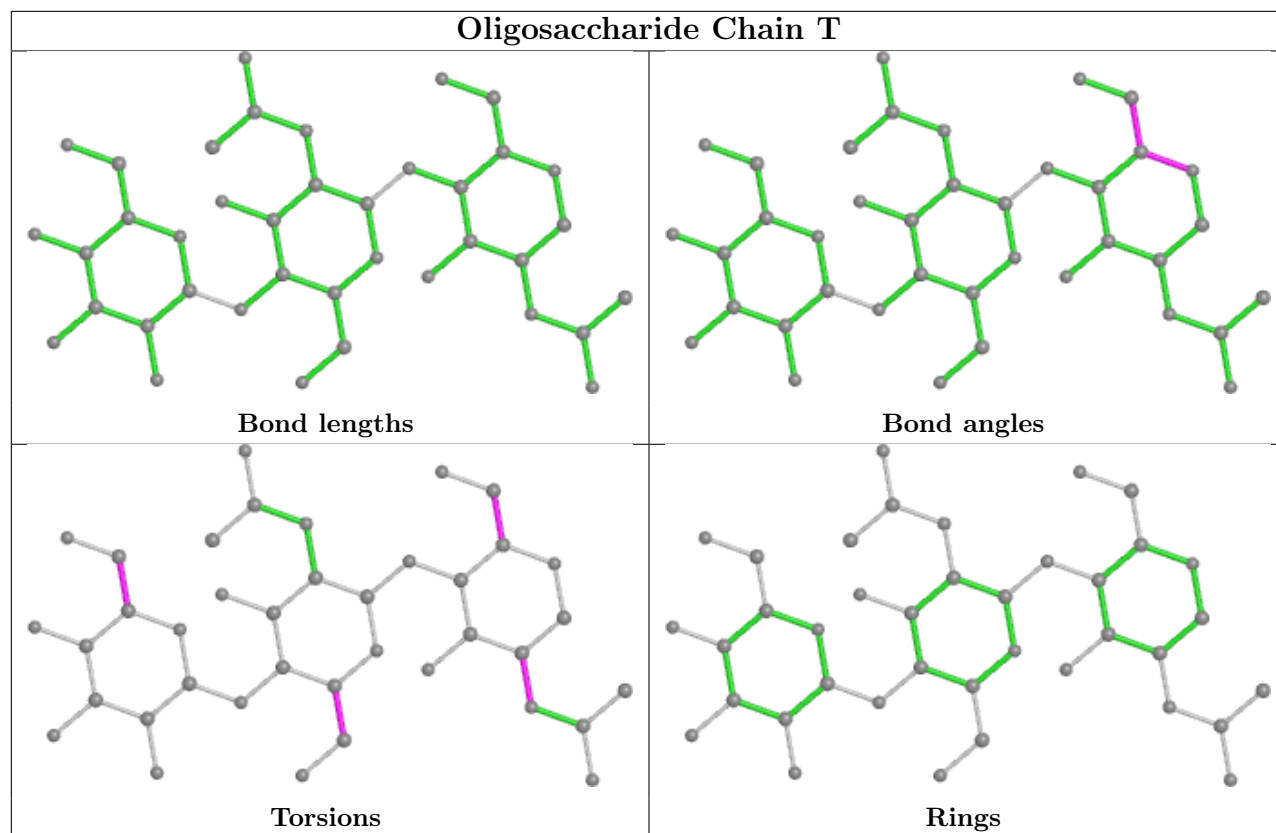


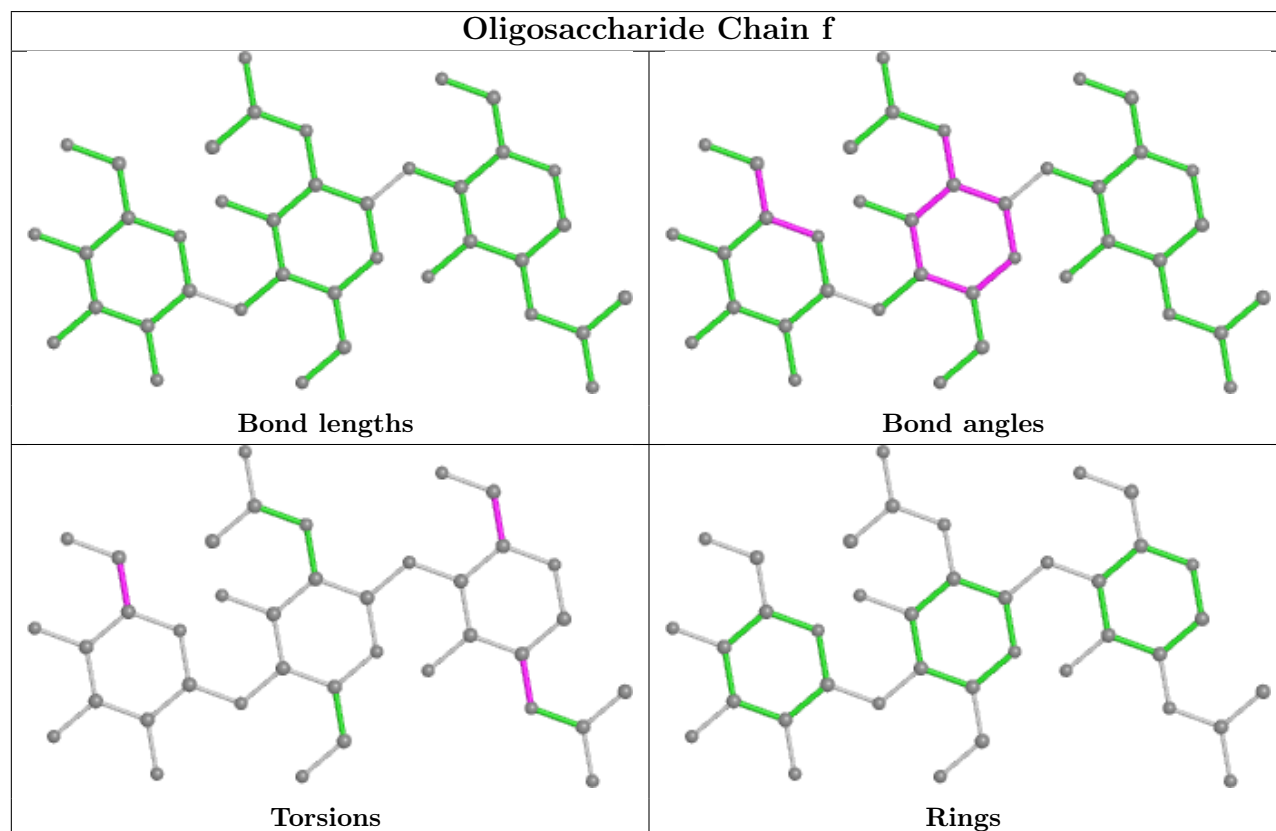
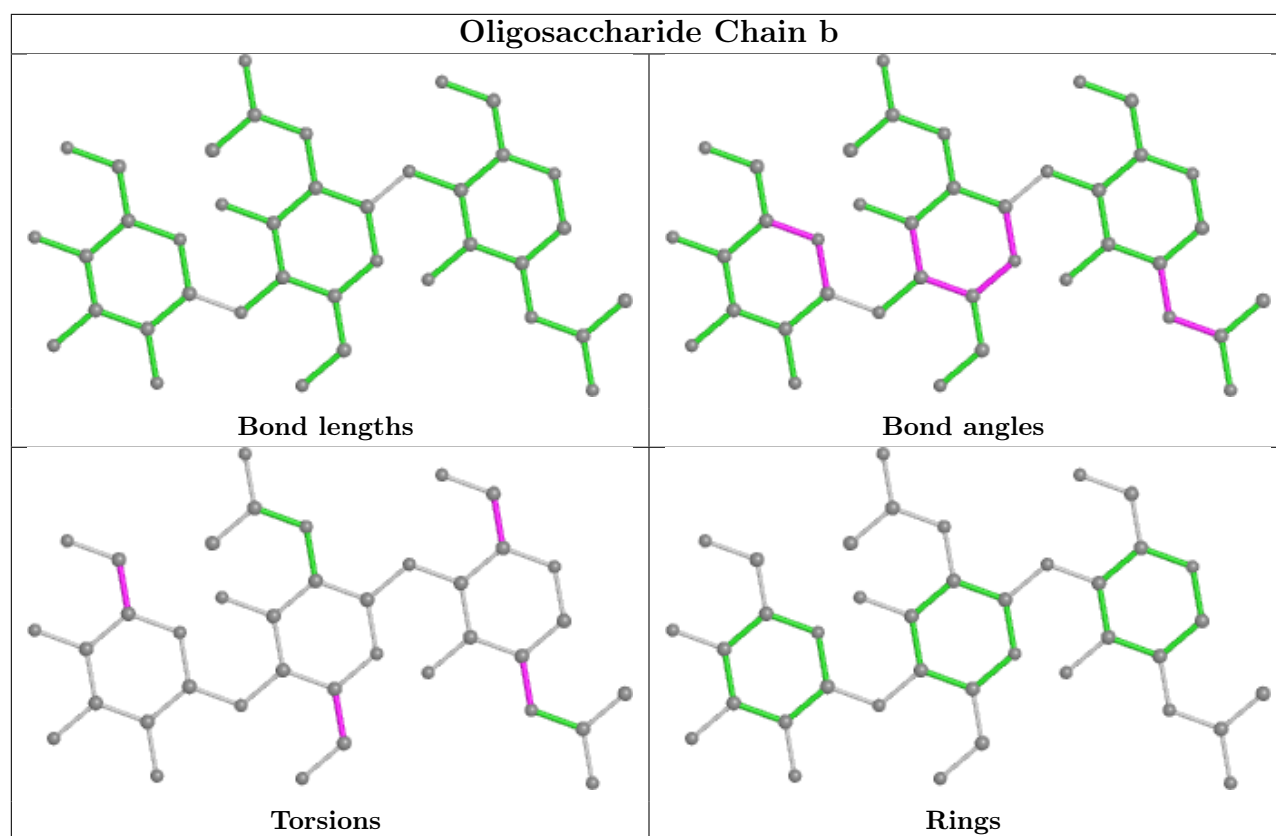


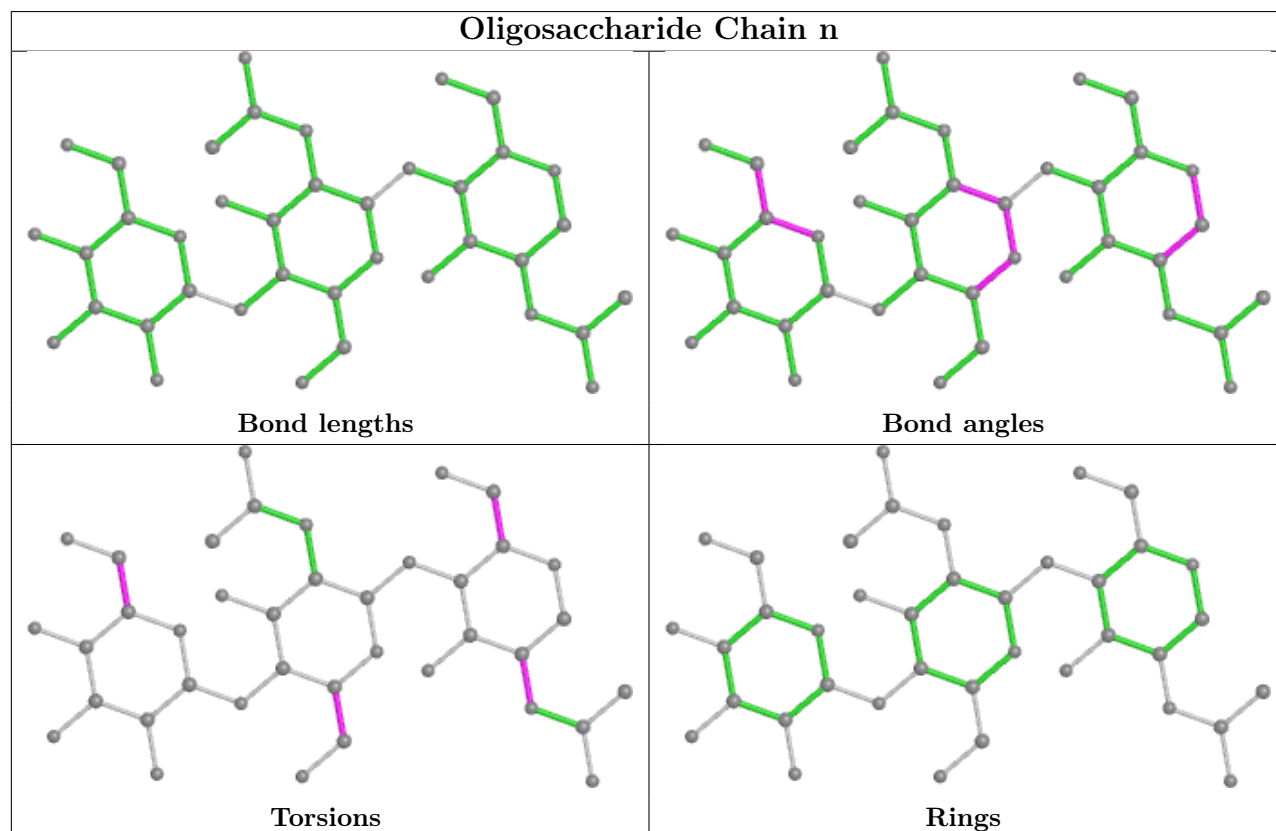
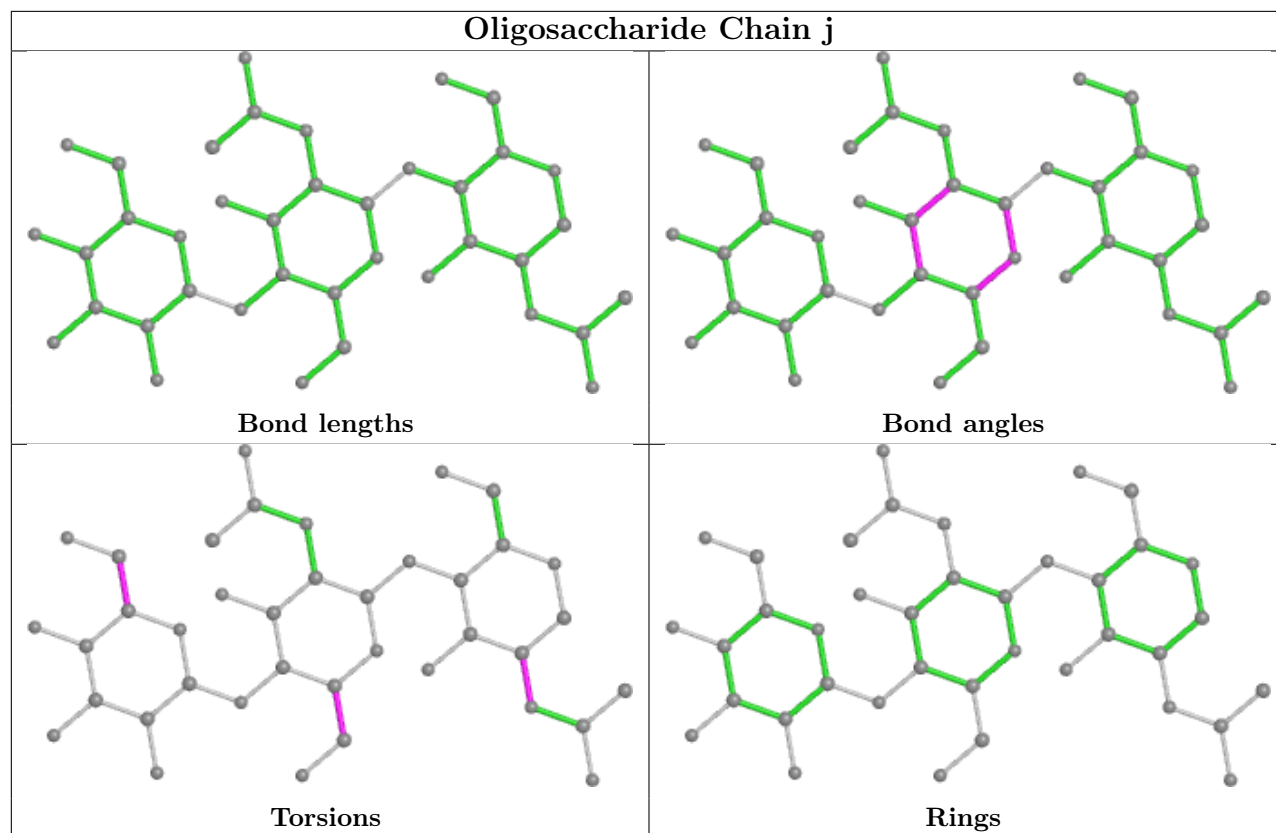


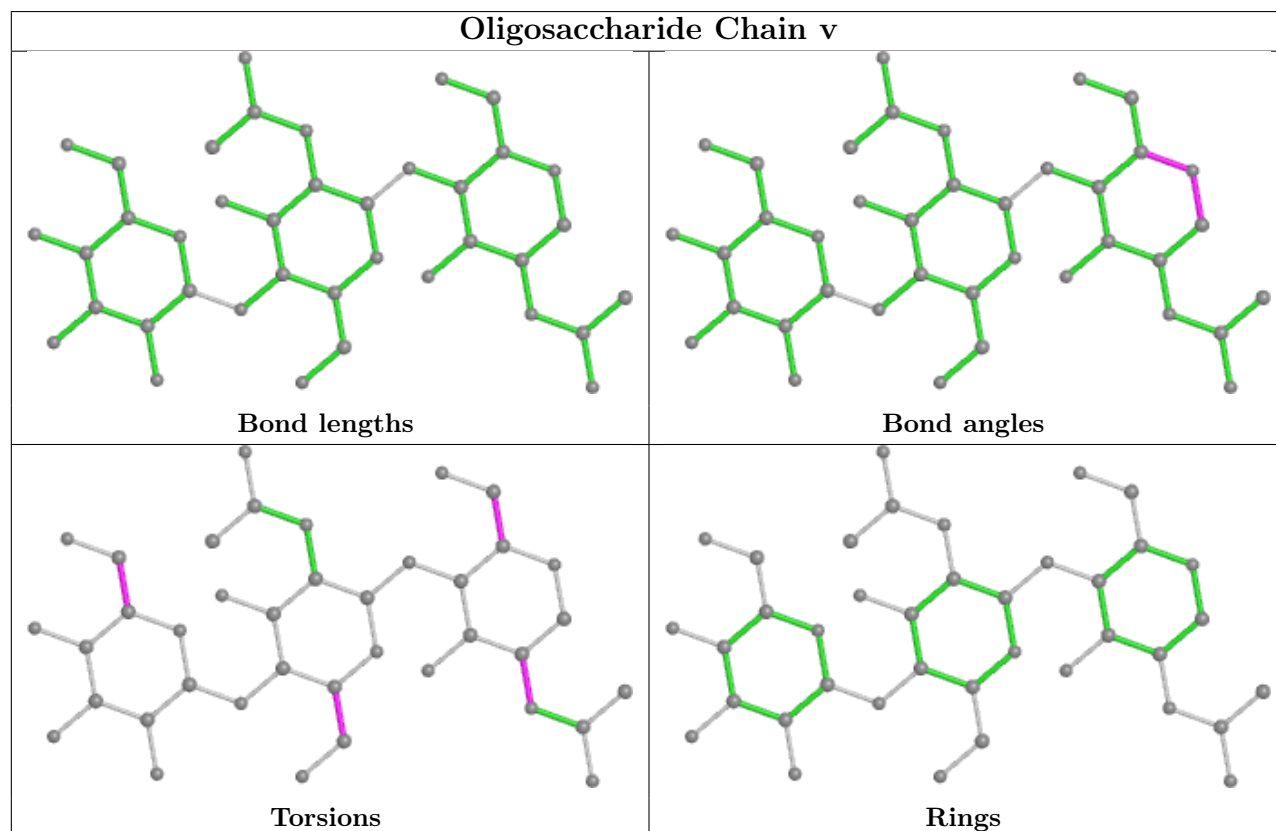
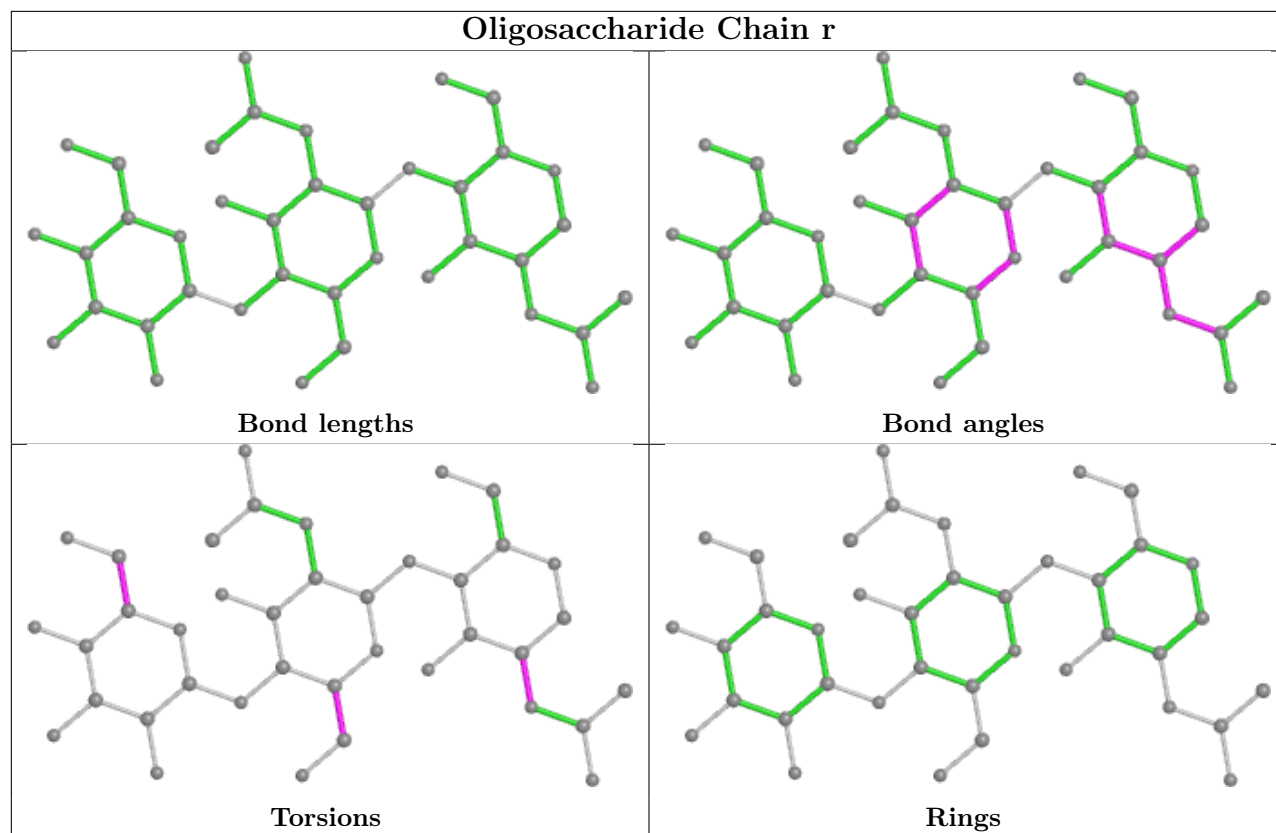












5.6 Ligand geometry

Of 73 ligands modelled in this entry, 8 are monoatomic - leaving 65 for Mogul analysis.

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	$\# Z > 2$
6	NAG	O	505	1	14,14,15	0.33	0	17,19,21	0.58	0
6	NAG	G	501	1	14,14,15	0.39	0	17,19,21	1.24	2 (11%)
6	NAG	C	503	1	14,14,15	0.38	0	17,19,21	0.86	1 (5%)
6	NAG	E	503	1	14,14,15	0.53	0	17,19,21	0.97	1 (5%)
6	NAG	G	504	1	14,14,15	0.30	0	17,19,21	0.79	0
6	NAG	K	501	1	14,14,15	0.26	0	17,19,21	0.74	0
6	NAG	M	505	1	14,14,15	0.35	0	17,19,21	0.99	2 (11%)
6	NAG	N	1002	2	14,14,15	0.37	0	17,19,21	0.87	0
6	NAG	J	1003	2	14,14,15	0.30	0	17,19,21	1.05	1 (5%)
6	NAG	N	1003	2	14,14,15	0.55	0	17,19,21	0.99	0
6	NAG	P	1004	2	14,14,15	0.36	0	17,19,21	0.92	1 (5%)
6	NAG	J	1004	2	14,14,15	0.46	0	17,19,21	0.93	1 (5%)
6	NAG	M	501	1	14,14,15	0.44	0	17,19,21	1.07	1 (5%)
8	GLC	L	1002	-	12,12,12	0.68	0	17,17,17	0.99	1 (5%)
6	NAG	C	505	1	14,14,15	0.26	0	17,19,21	0.76	0
6	NAG	K	503	1	14,14,15	0.35	0	17,19,21	1.29	2 (11%)
6	NAG	E	502	1	14,14,15	0.27	0	17,19,21	0.63	0
6	NAG	M	504	1	14,14,15	0.35	0	17,19,21	1.18	1 (5%)
6	NAG	B	1003	2	14,14,15	0.35	0	17,19,21	0.76	0
6	NAG	P	1003	2	14,14,15	0.40	0	17,19,21	0.93	1 (5%)
6	NAG	C	501	1	14,14,15	0.34	0	17,19,21	0.79	1 (5%)
6	NAG	O	502	1	14,14,15	0.31	0	17,19,21	0.72	0
6	NAG	F	1002	2	14,14,15	0.37	0	17,19,21	0.94	1 (5%)
6	NAG	A	503	1	14,14,15	0.37	0	17,19,21	0.92	0
8	GLC	I	506	-	12,12,12	0.58	0	17,17,17	0.54	0
6	NAG	O	503	1	14,14,15	0.42	0	17,19,21	0.89	2 (11%)
6	NAG	I	501	1	14,14,15	0.40	0	17,19,21	0.96	1 (5%)
6	NAG	A	505	1	14,14,15	0.40	0	17,19,21	1.11	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GLC	E	506	-	12,12,12	0.63	0	17,17,17	0.78	0
8	GLC	G	506	-	12,12,12	0.60	0	17,17,17	0.78	0
6	NAG	E	505	1	14,14,15	0.28	0	17,19,21	0.74	0
6	NAG	I	504	1	14,14,15	0.27	0	17,19,21	1.12	2 (11%)
6	NAG	H	1002	2	14,14,15	0.37	0	17,19,21	0.72	0
8	GLC	B	1002	-	12,12,12	0.64	0	17,17,17	0.81	1 (5%)
8	GLC	P	1002	-	12,12,12	0.57	0	17,17,17	0.66	0
6	NAG	G	502	1	14,14,15	0.26	0	17,19,21	0.61	0
6	NAG	H	1003	2	14,14,15	0.29	0	17,19,21	0.88	1 (5%)
6	NAG	H	1004	2	14,14,15	0.44	0	17,19,21	0.85	1 (5%)
6	NAG	M	502	1	14,14,15	0.28	0	17,19,21	0.92	1 (5%)
6	NAG	I	505	1	14,14,15	0.32	0	17,19,21	0.64	0
6	NAG	A	501	1	14,14,15	0.35	0	17,19,21	0.66	0
6	NAG	I	503	1	14,14,15	0.35	0	17,19,21	1.06	1 (5%)
6	NAG	J	1002	2	14,14,15	0.37	0	17,19,21	0.69	0
6	NAG	D	1002	2	14,14,15	0.34	0	17,19,21	0.91	1 (5%)
6	NAG	G	505	1	14,14,15	0.40	0	17,19,21	1.12	2 (11%)
6	NAG	C	502	1	14,14,15	0.30	0	17,19,21	0.73	1 (5%)
6	NAG	C	504	1	14,14,15	0.37	0	17,19,21	1.12	2 (11%)
6	NAG	O	501	1	14,14,15	0.41	0	17,19,21	0.98	1 (5%)
6	NAG	O	504	1	14,14,15	0.36	0	17,19,21	1.10	1 (5%)
6	NAG	D	1003	2	14,14,15	0.34	0	17,19,21	0.98	2 (11%)
6	NAG	E	501	1	14,14,15	0.54	0	17,19,21	0.93	0
6	NAG	B	1004	2	14,14,15	0.46	0	17,19,21	0.62	0
6	NAG	I	502	1	14,14,15	0.32	0	17,19,21	0.56	0
6	NAG	L	1005	2	14,14,15	0.50	0	17,19,21	1.81	5 (29%)
6	NAG	E	504	1	14,14,15	0.31	0	17,19,21	0.89	1 (5%)
8	GLC	M	506	-	12,12,12	0.54	0	17,17,17	0.62	0
6	NAG	G	503	1	14,14,15	0.45	0	17,19,21	1.23	2 (11%)
6	NAG	A	504	1	14,14,15	0.45	0	17,19,21	0.99	1 (5%)
6	NAG	K	502	1	14,14,15	0.34	0	17,19,21	0.89	0
6	NAG	F	1003	2	14,14,15	0.45	0	17,19,21	0.67	0
8	GLC	C	506	-	12,12,12	0.58	0	17,17,17	0.69	0
6	NAG	L	1003	2	14,14,15	0.42	0	17,19,21	1.10	2 (11%)
6	NAG	L	1004	2	14,14,15	0.37	0	17,19,21	0.65	0
6	NAG	A	502	1	14,14,15	0.25	0	17,19,21	0.87	1 (5%)
6	NAG	M	503	1	14,14,15	0.36	0	17,19,21	1.06	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	O	505	1	-	1/6/23/26	0/1/1/1
6	NAG	G	501	1	-	2/6/23/26	0/1/1/1
6	NAG	C	503	1	-	2/6/23/26	0/1/1/1
6	NAG	E	503	1	-	0/6/23/26	0/1/1/1
6	NAG	G	504	1	-	0/6/23/26	0/1/1/1
6	NAG	K	501	1	-	0/6/23/26	0/1/1/1
6	NAG	M	505	1	-	1/6/23/26	0/1/1/1
6	NAG	N	1002	2	-	0/6/23/26	0/1/1/1
6	NAG	J	1003	2	-	0/6/23/26	0/1/1/1
6	NAG	N	1003	2	-	2/6/23/26	0/1/1/1
6	NAG	P	1004	2	-	0/6/23/26	0/1/1/1
6	NAG	J	1004	2	-	2/6/23/26	0/1/1/1
6	NAG	M	501	1	-	3/6/23/26	0/1/1/1
8	GLC	L	1002	-	-	0/2/22/22	0/1/1/1
6	NAG	C	505	1	-	2/6/23/26	0/1/1/1
6	NAG	K	503	1	-	0/6/23/26	0/1/1/1
6	NAG	E	502	1	-	0/6/23/26	0/1/1/1
6	NAG	M	504	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1003	2	-	0/6/23/26	0/1/1/1
6	NAG	P	1003	2	-	0/6/23/26	0/1/1/1
6	NAG	C	501	1	-	2/6/23/26	0/1/1/1
6	NAG	O	502	1	-	2/6/23/26	0/1/1/1
6	NAG	F	1002	2	-	0/6/23/26	0/1/1/1
6	NAG	A	503	1	-	1/6/23/26	0/1/1/1
8	GLC	I	506	-	-	2/2/22/22	0/1/1/1
6	NAG	O	503	1	-	2/6/23/26	0/1/1/1
6	NAG	I	501	1	-	4/6/23/26	0/1/1/1
6	NAG	A	505	1	-	0/6/23/26	0/1/1/1
8	GLC	E	506	-	-	2/2/22/22	0/1/1/1
8	GLC	G	506	-	-	0/2/22/22	0/1/1/1
6	NAG	E	505	1	-	0/6/23/26	0/1/1/1
6	NAG	I	504	1	-	0/6/23/26	0/1/1/1
6	NAG	H	1002	2	-	0/6/23/26	0/1/1/1
8	GLC	B	1002	-	-	0/2/22/22	0/1/1/1
8	GLC	P	1002	-	-	0/2/22/22	0/1/1/1
6	NAG	G	502	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	H	1003	2	-	2/6/23/26	0/1/1/1
6	NAG	H	1004	2	-	0/6/23/26	0/1/1/1
6	NAG	M	502	1	-	0/6/23/26	0/1/1/1
6	NAG	I	505	1	-	2/6/23/26	0/1/1/1
6	NAG	A	501	1	-	0/6/23/26	0/1/1/1
6	NAG	I	503	1	-	0/6/23/26	0/1/1/1
6	NAG	J	1002	2	-	0/6/23/26	0/1/1/1
6	NAG	D	1002	2	-	0/6/23/26	0/1/1/1
6	NAG	G	505	1	-	0/6/23/26	0/1/1/1
6	NAG	C	502	1	-	0/6/23/26	0/1/1/1
6	NAG	C	504	1	-	2/6/23/26	0/1/1/1
6	NAG	O	501	1	-	1/6/23/26	0/1/1/1
6	NAG	O	504	1	-	0/6/23/26	0/1/1/1
6	NAG	D	1003	2	-	0/6/23/26	0/1/1/1
6	NAG	E	501	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1004	2	-	0/6/23/26	0/1/1/1
6	NAG	I	502	1	-	0/6/23/26	0/1/1/1
6	NAG	L	1005	2	-	0/6/23/26	0/1/1/1
6	NAG	E	504	1	-	0/6/23/26	0/1/1/1
8	GLC	M	506	-	-	1/2/22/22	0/1/1/1
6	NAG	G	503	1	-	2/6/23/26	0/1/1/1
6	NAG	A	504	1	-	0/6/23/26	0/1/1/1
6	NAG	K	502	1	-	0/6/23/26	0/1/1/1
6	NAG	F	1003	2	-	0/6/23/26	0/1/1/1
8	GLC	C	506	-	-	0/2/22/22	0/1/1/1
6	NAG	L	1003	2	-	0/6/23/26	0/1/1/1
6	NAG	L	1004	2	-	0/6/23/26	0/1/1/1
6	NAG	A	502	1	-	0/6/23/26	0/1/1/1
6	NAG	M	503	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1005	NAG	C1-O5-C5	5.21	119.25	112.19
6	G	503	NAG	C1-O5-C5	4.10	117.75	112.19
6	O	504	NAG	C1-O5-C5	3.85	117.41	112.19
6	K	503	NAG	C1-O5-C5	3.34	116.72	112.19
6	I	504	NAG	C1-O5-C5	3.29	116.64	112.19

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

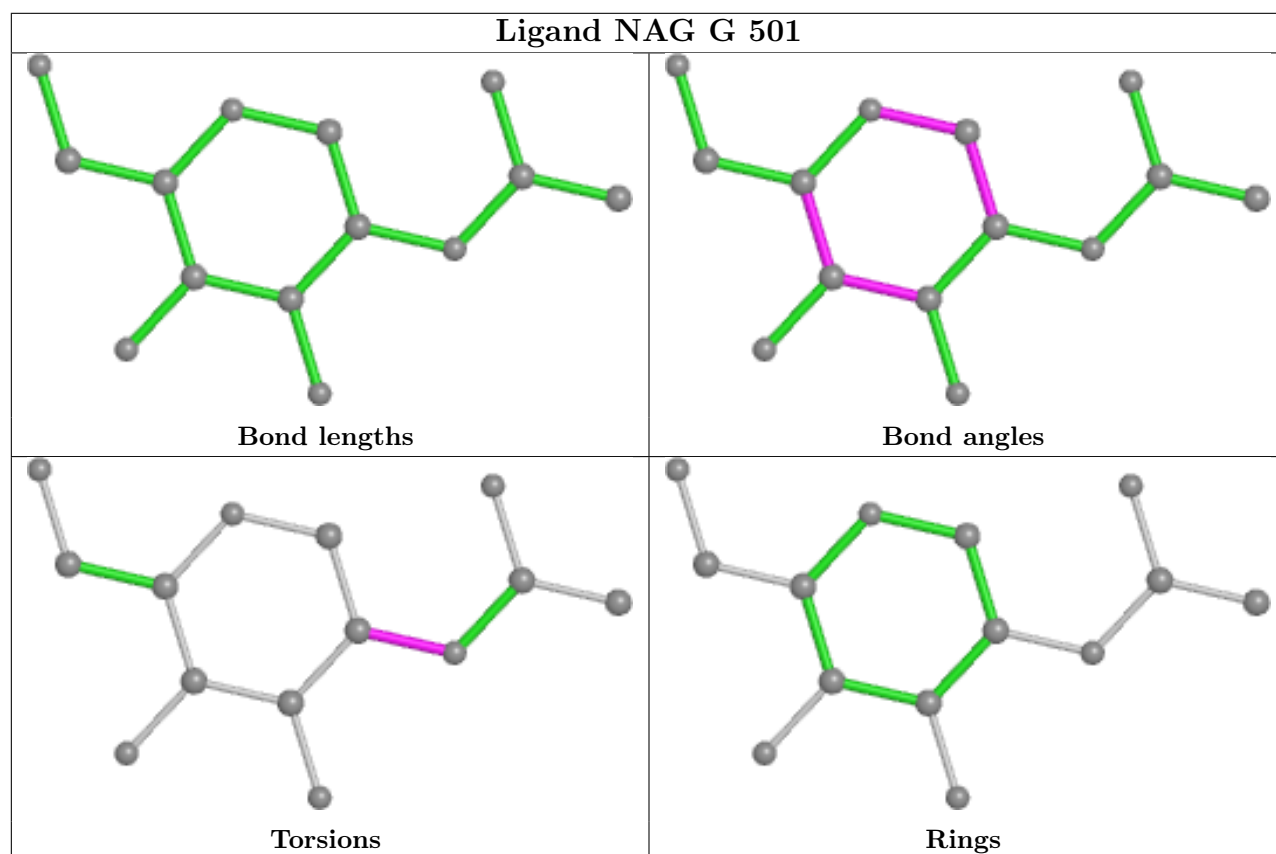
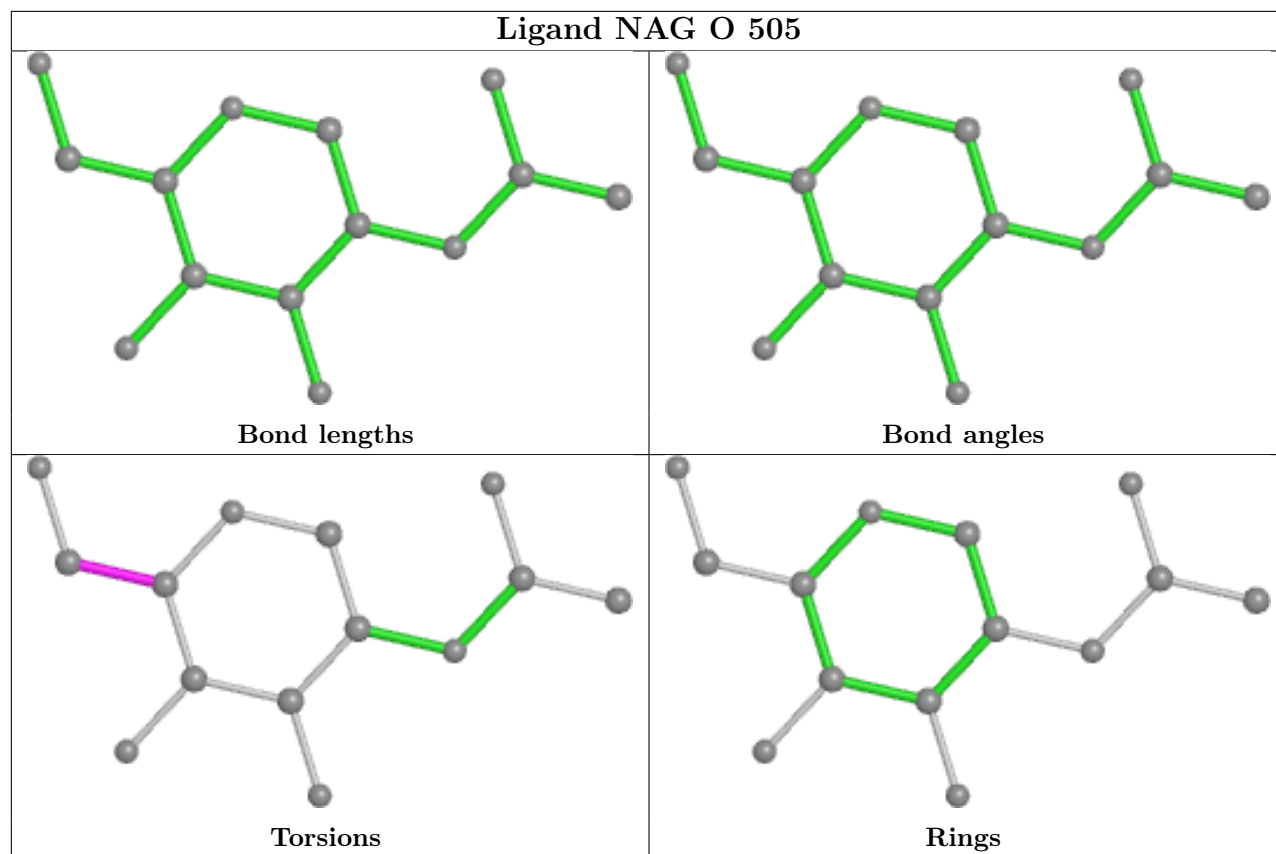
Mol	Chain	Res	Type	Atoms
6	C	503	NAG	O5-C5-C6-O6
6	O	503	NAG	O5-C5-C6-O6
6	G	503	NAG	O5-C5-C6-O6
6	C	503	NAG	C4-C5-C6-O6
6	C	501	NAG	O5-C5-C6-O6

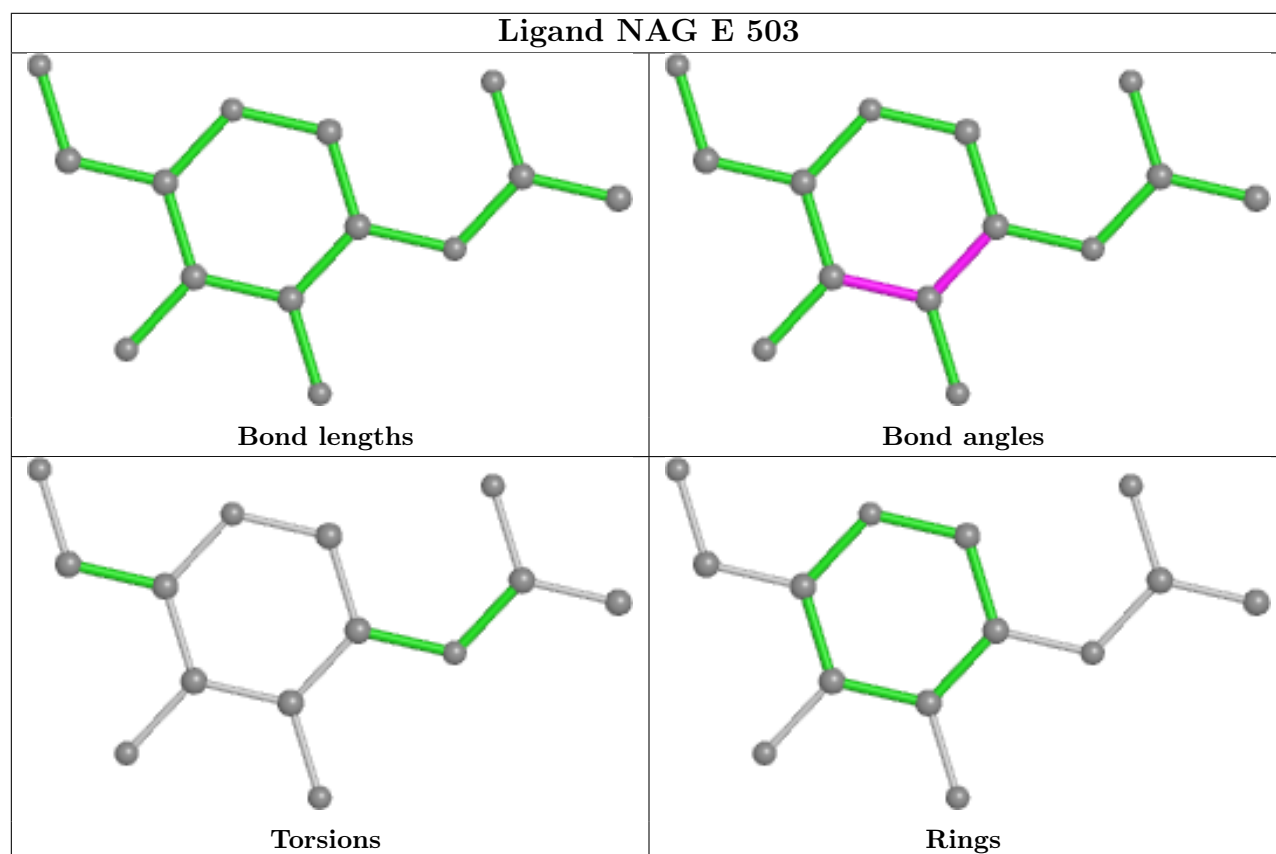
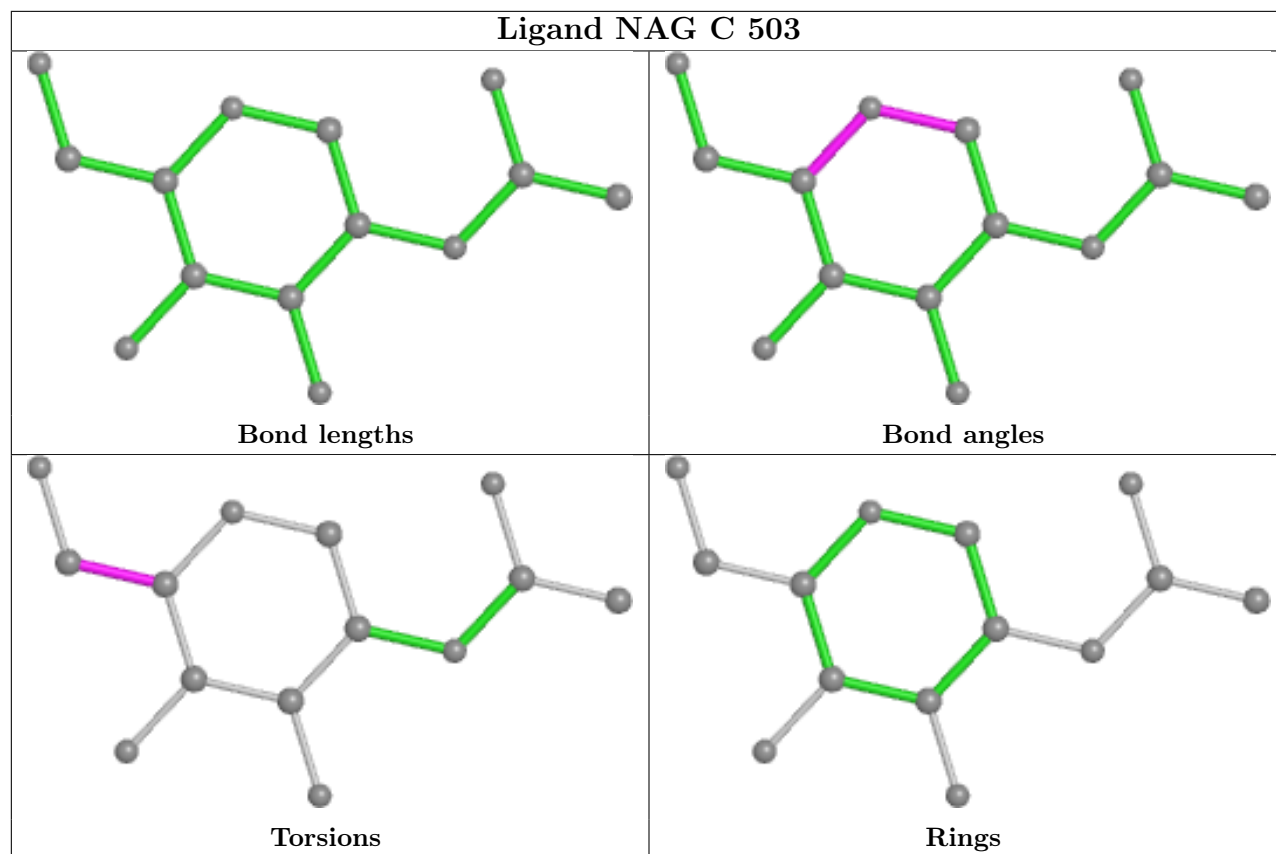
There are no ring outliers.

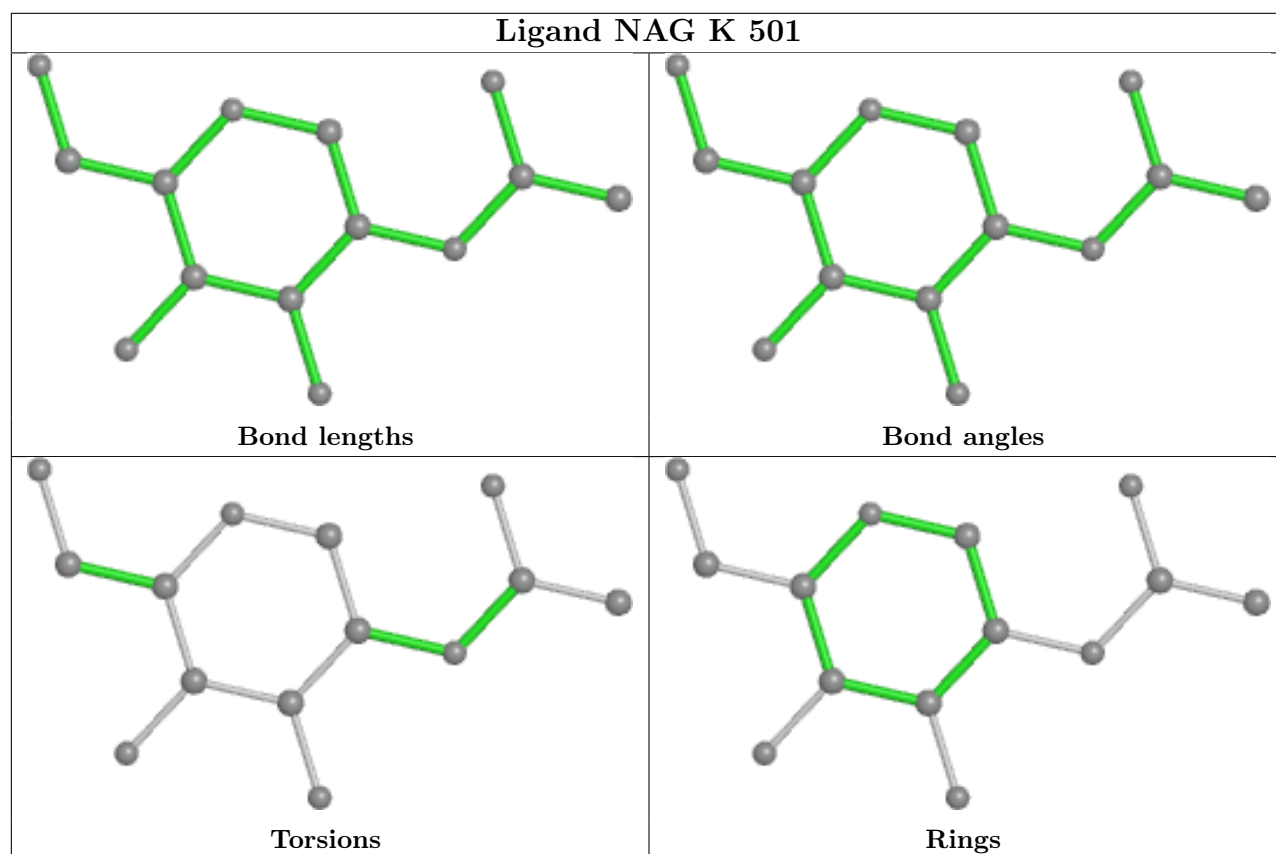
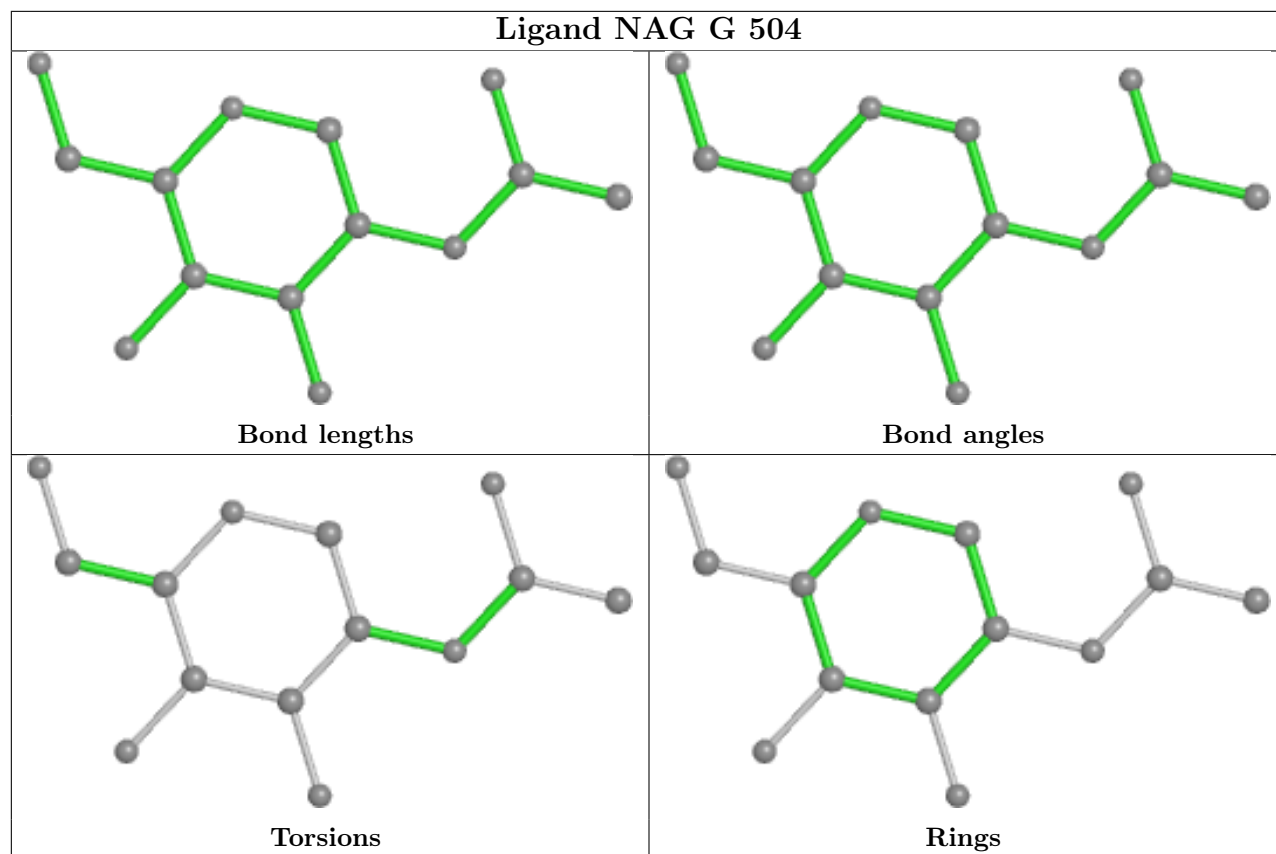
1 monomer is involved in 1 short contact:

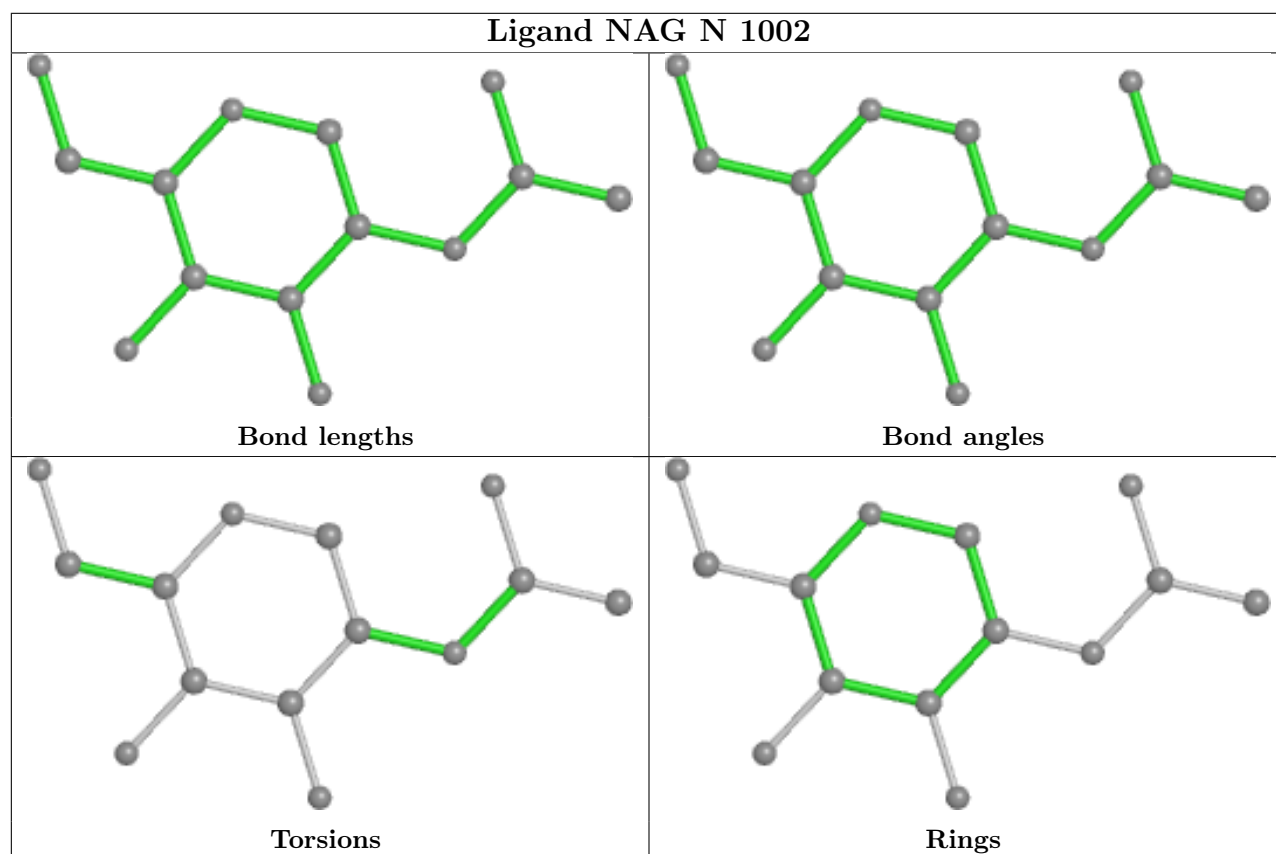
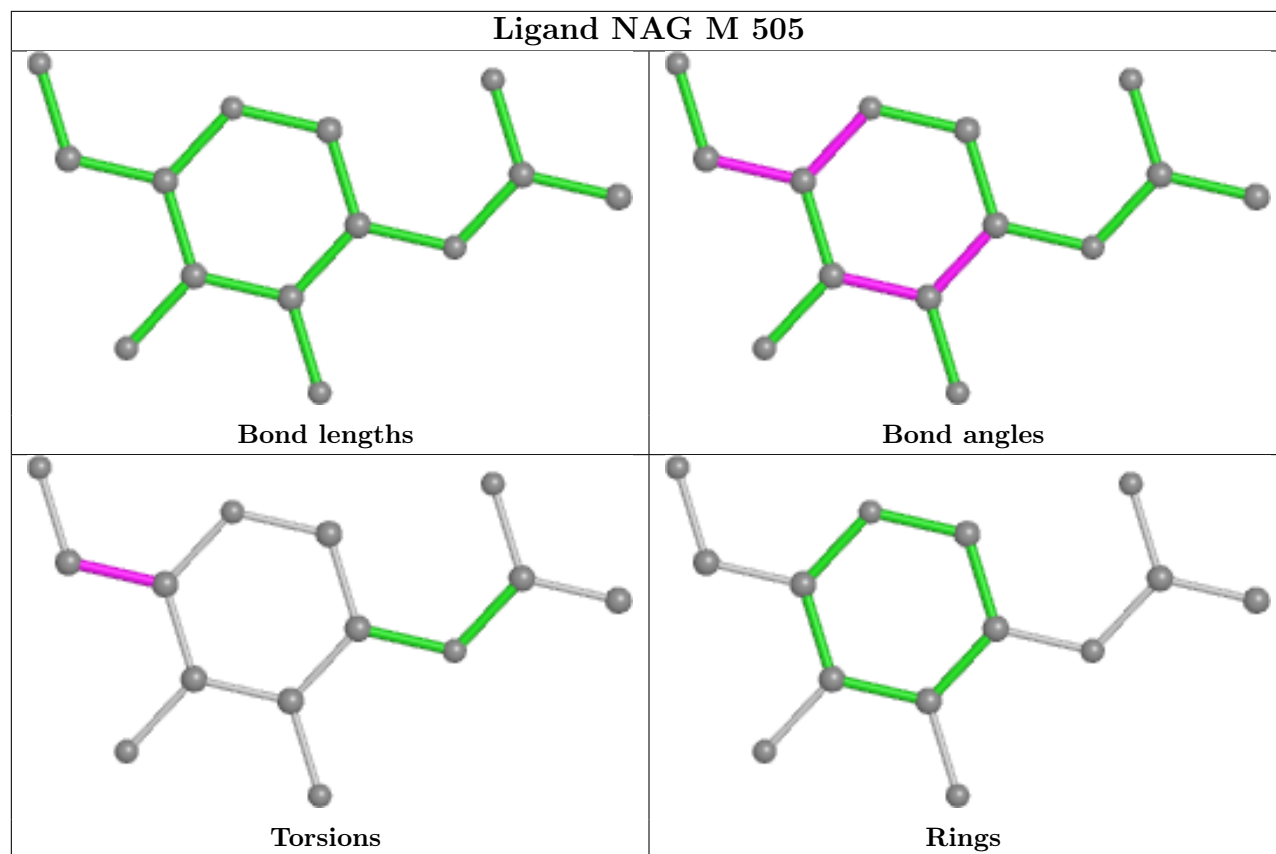
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	504	NAG	1	0

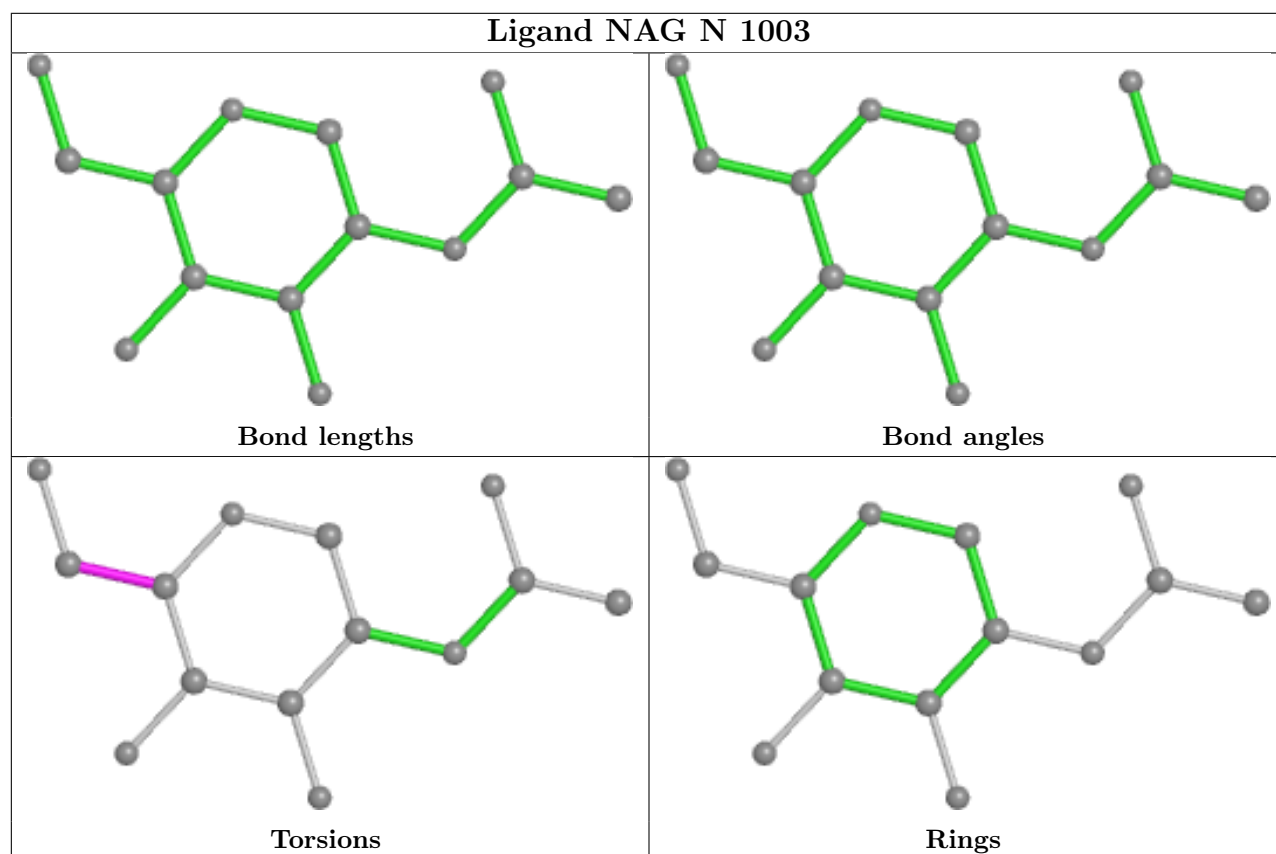
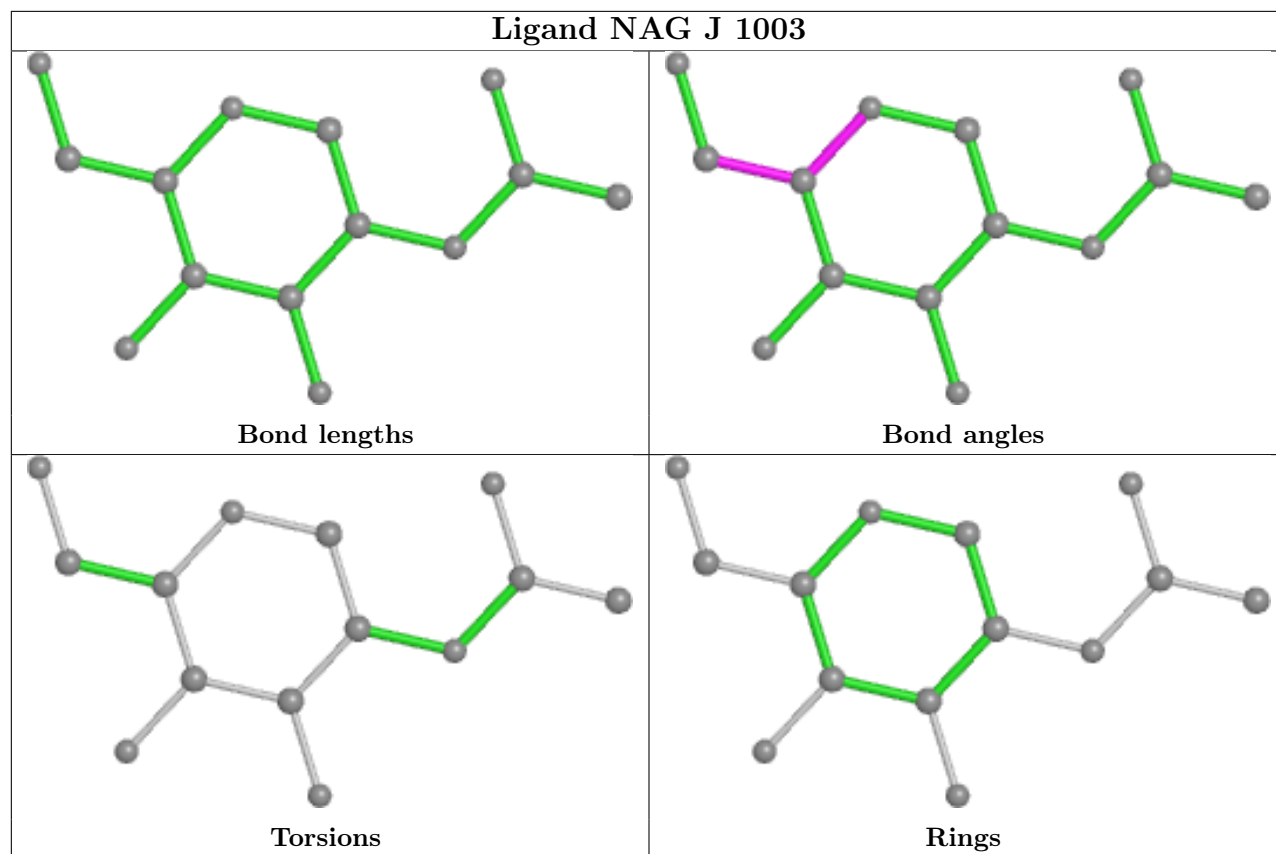
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

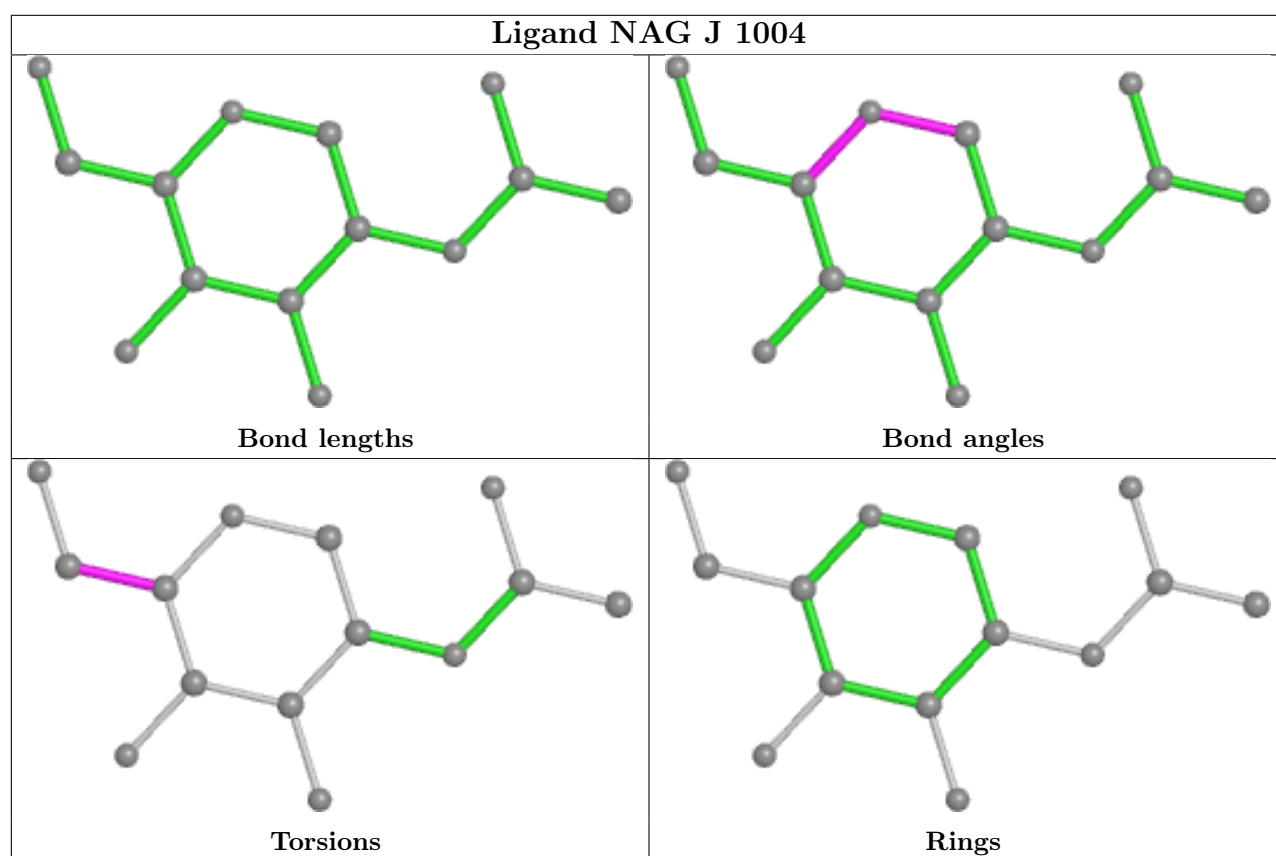
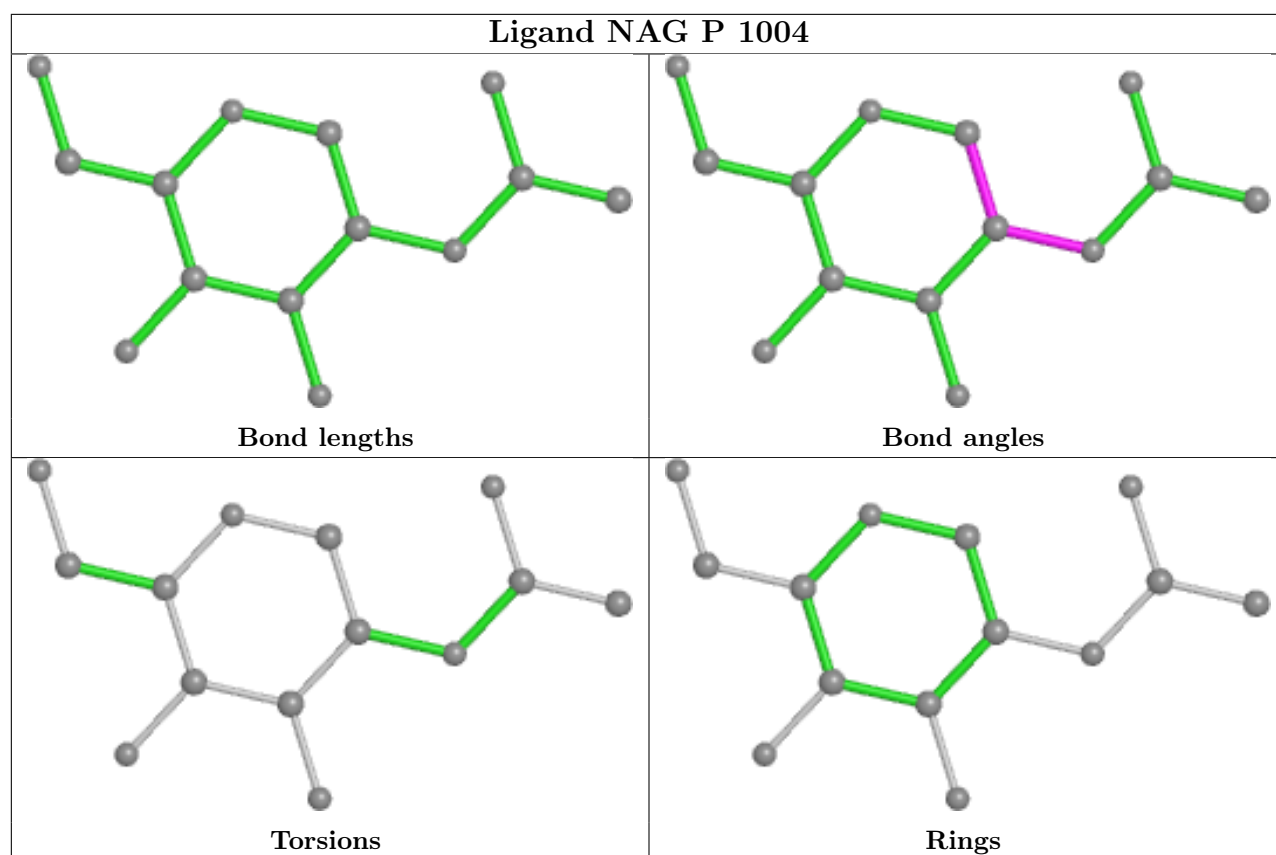


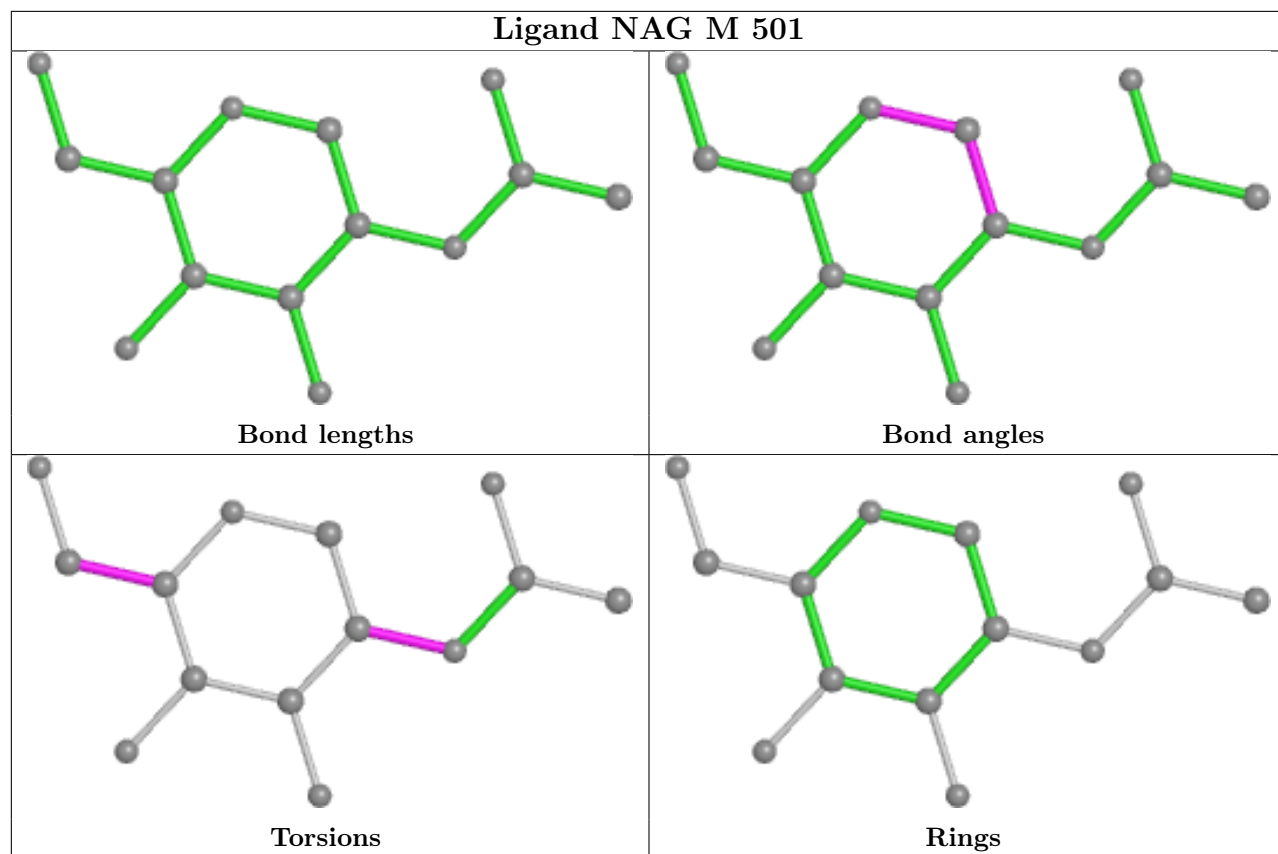


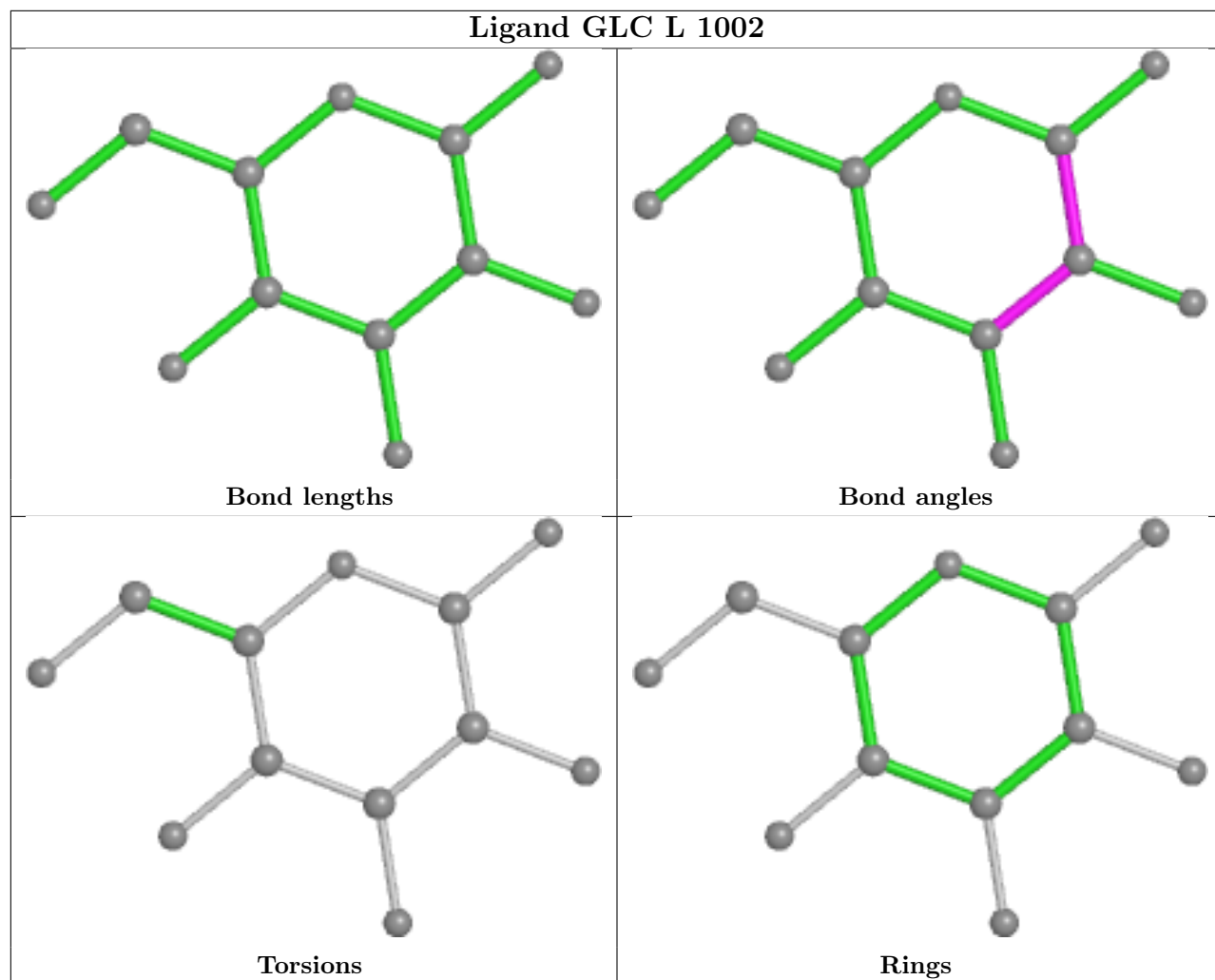


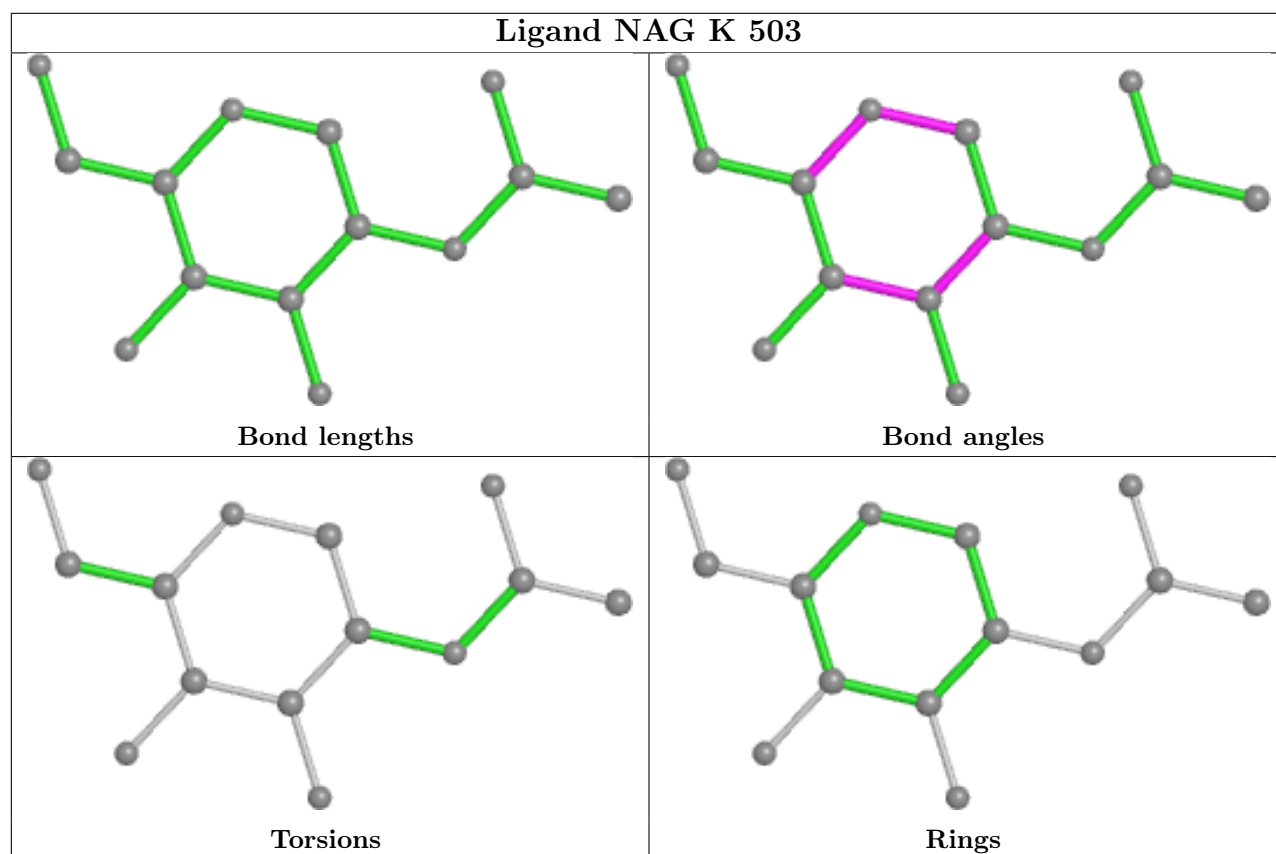
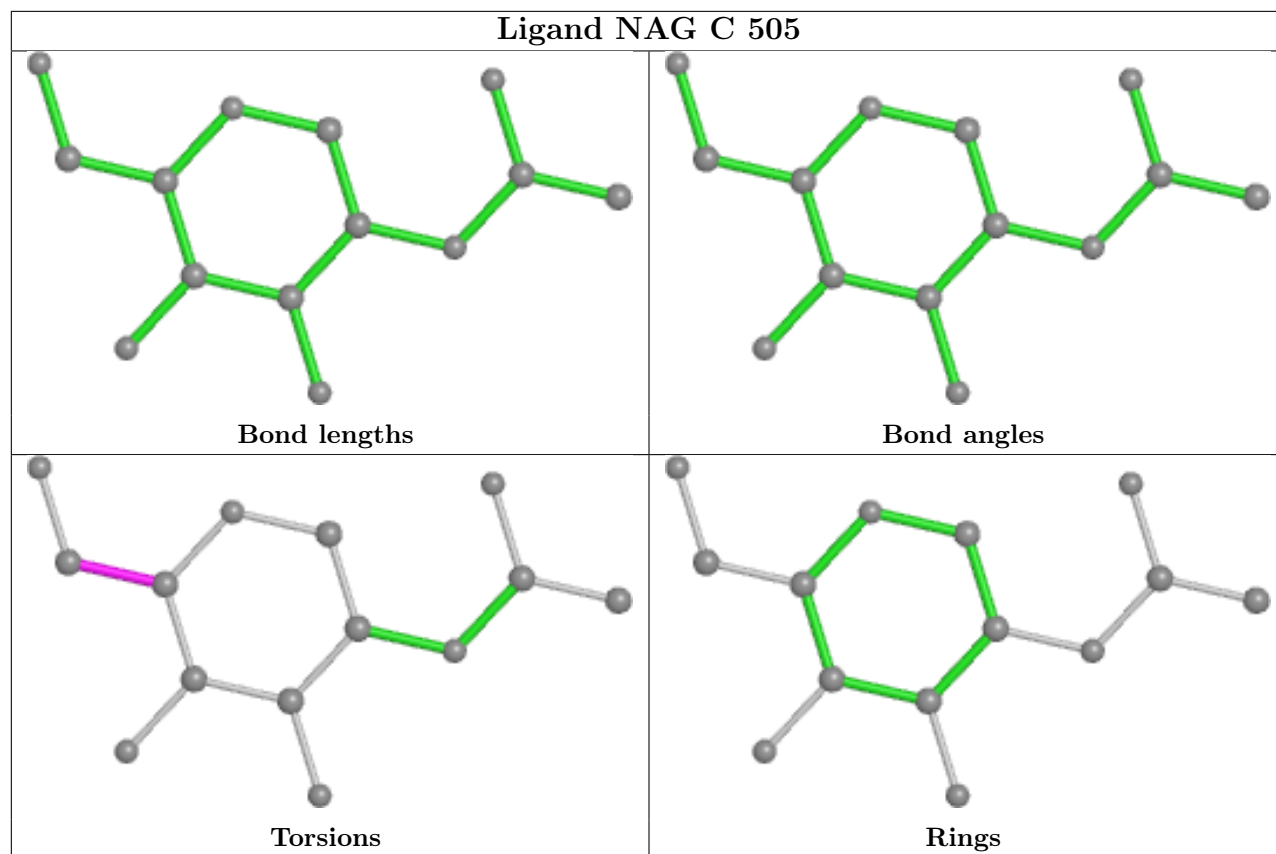


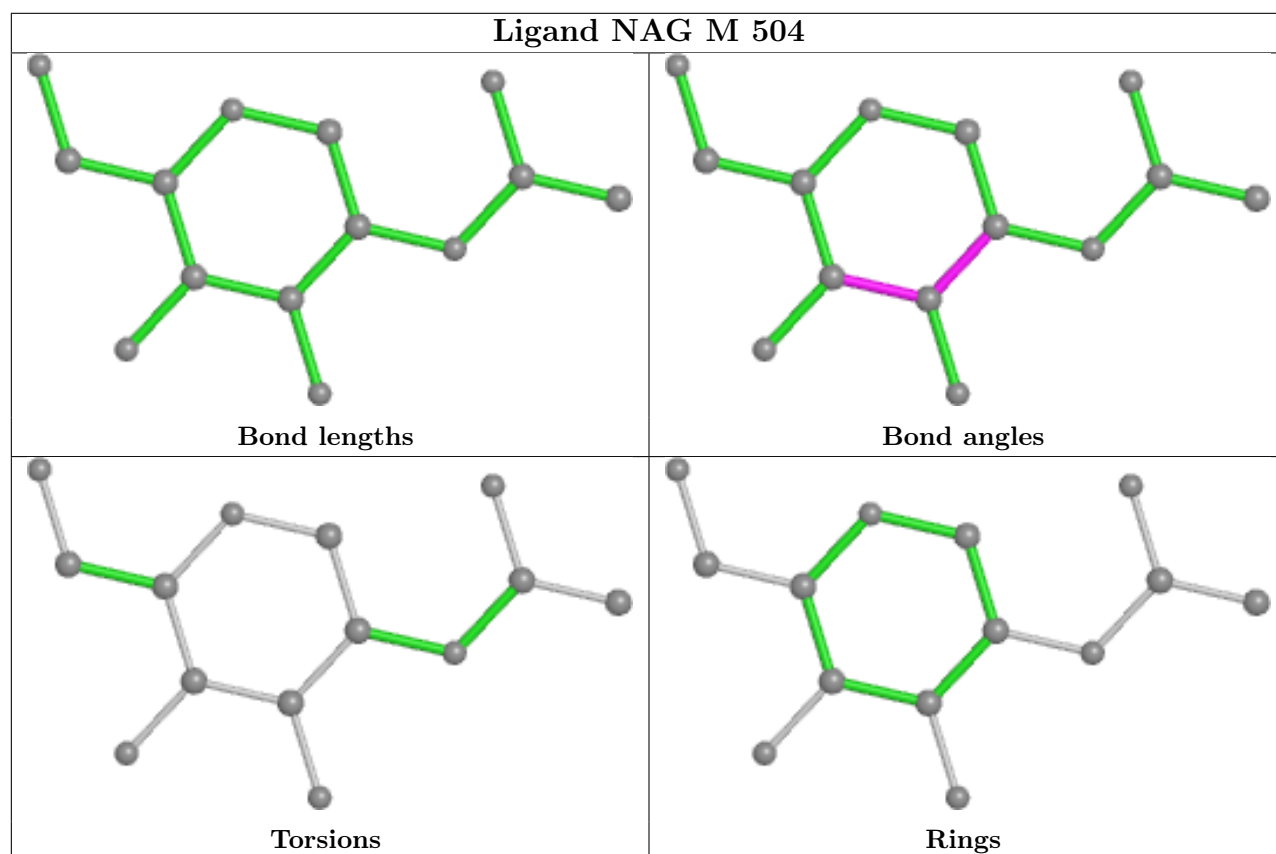
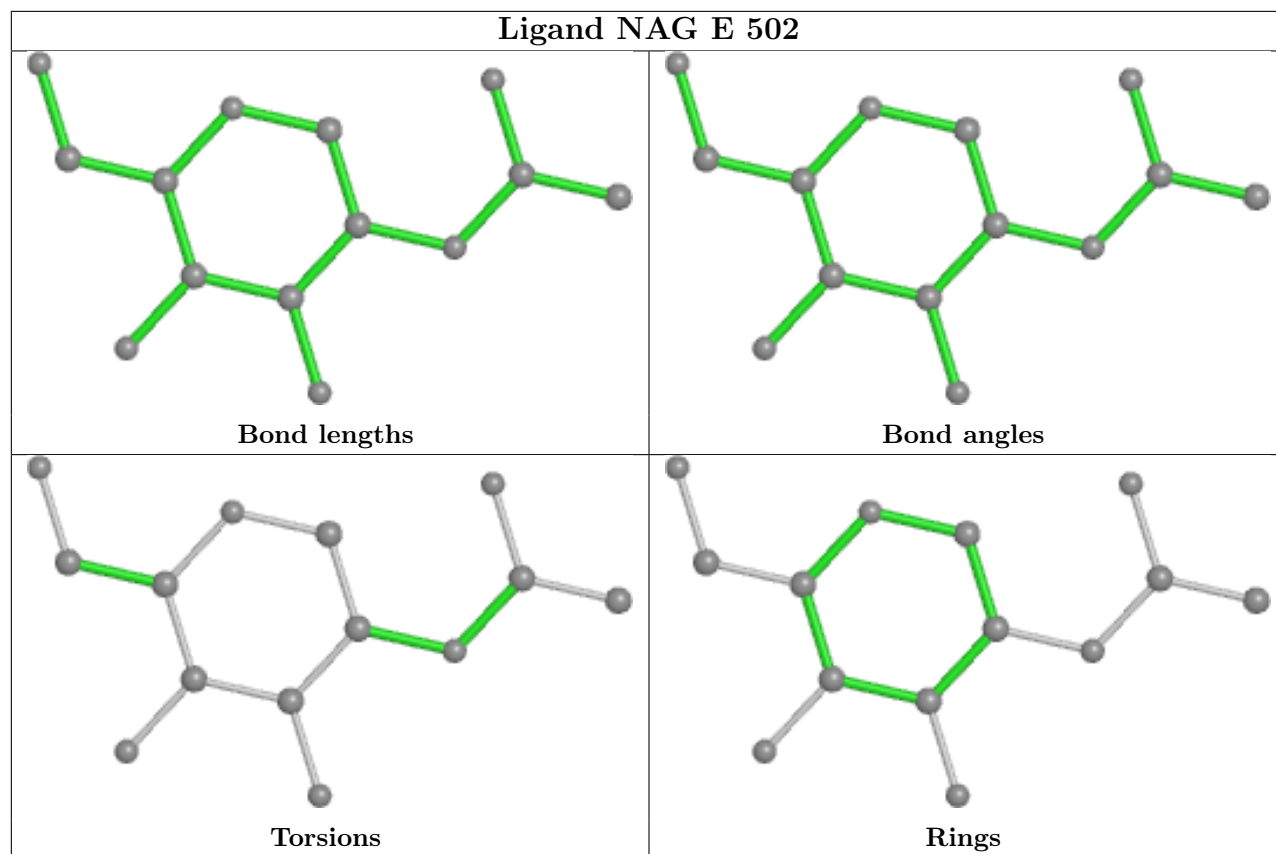


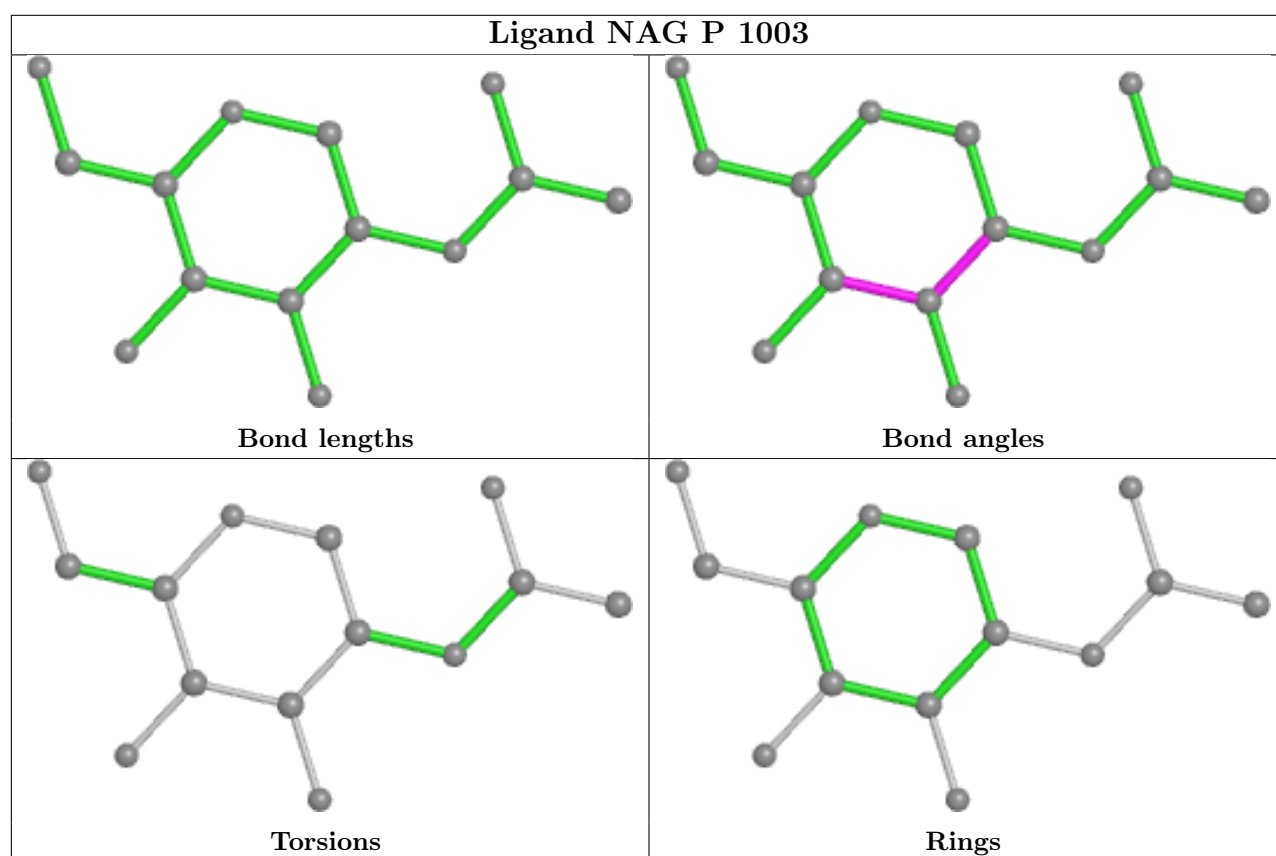
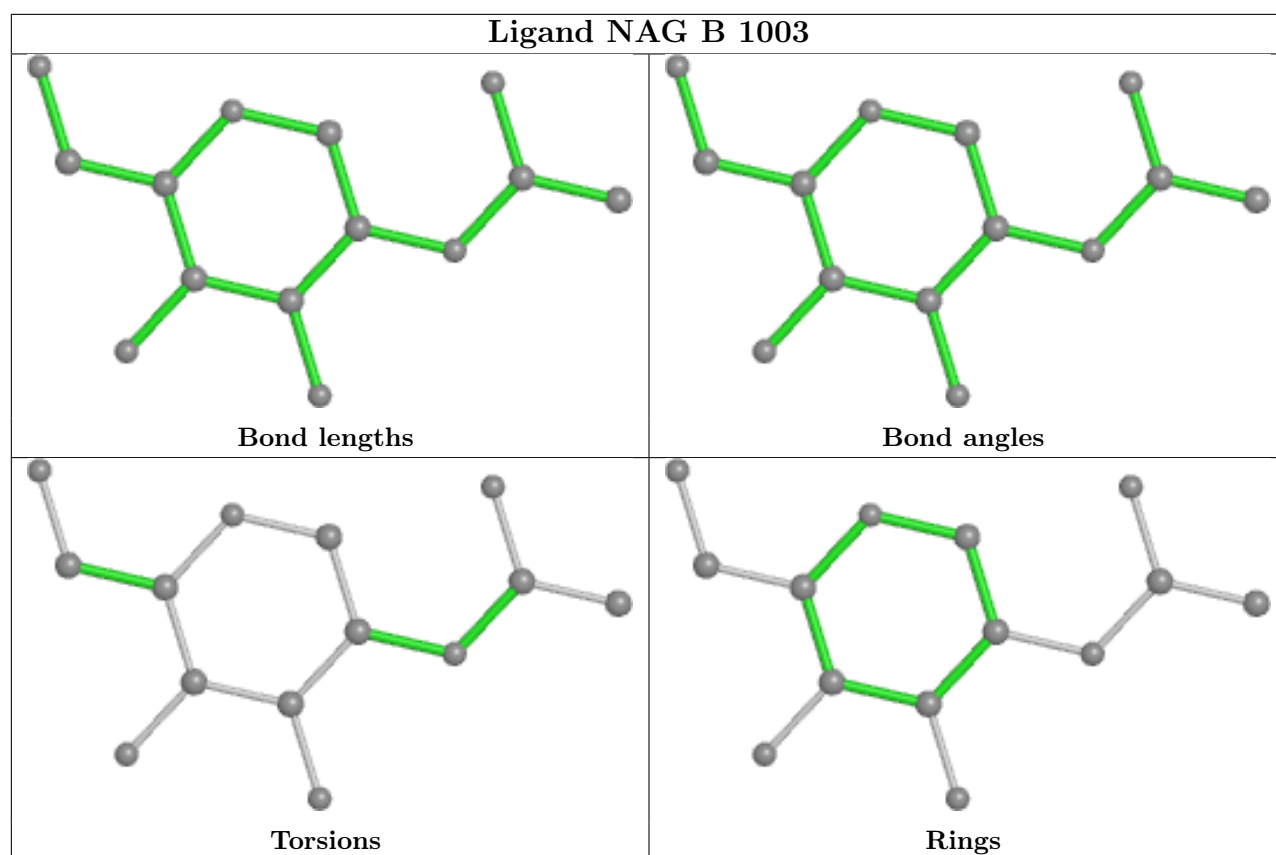


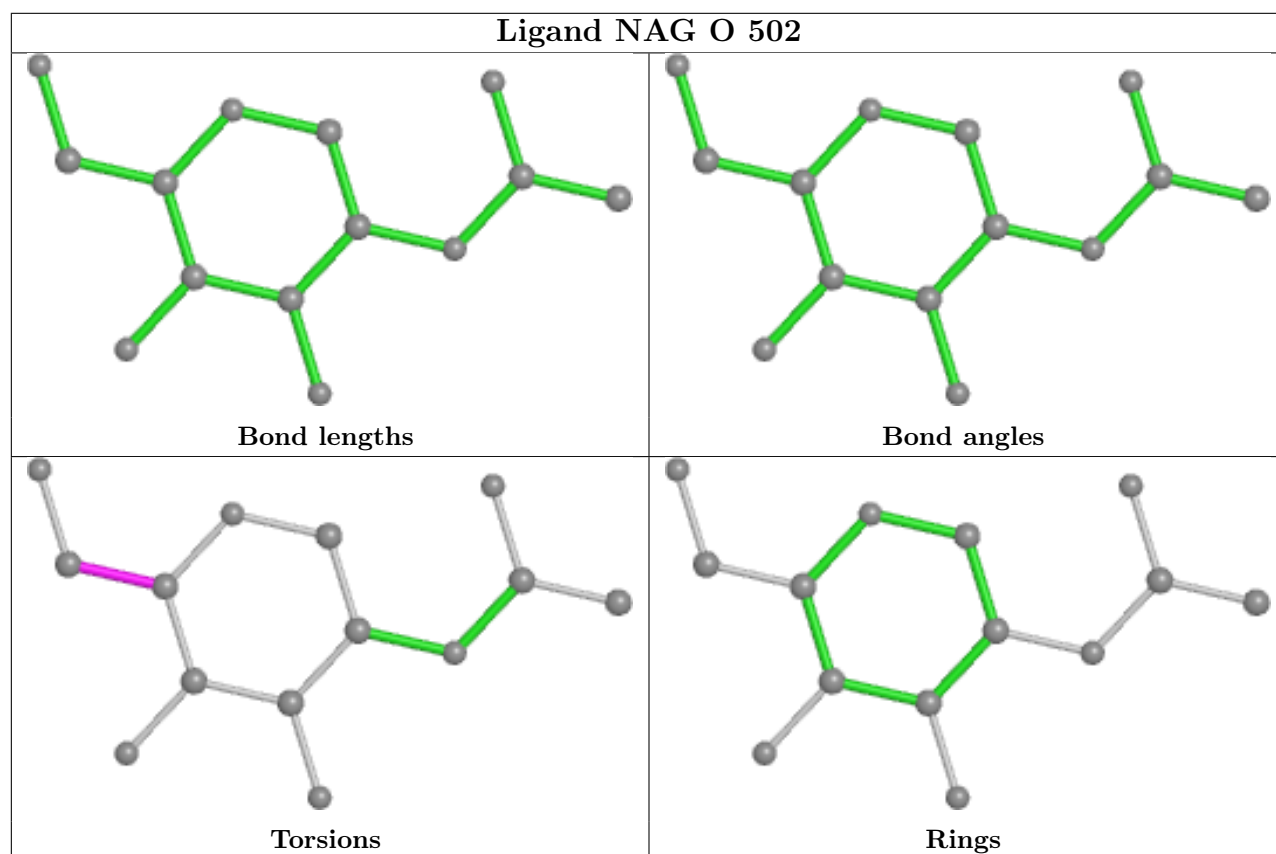
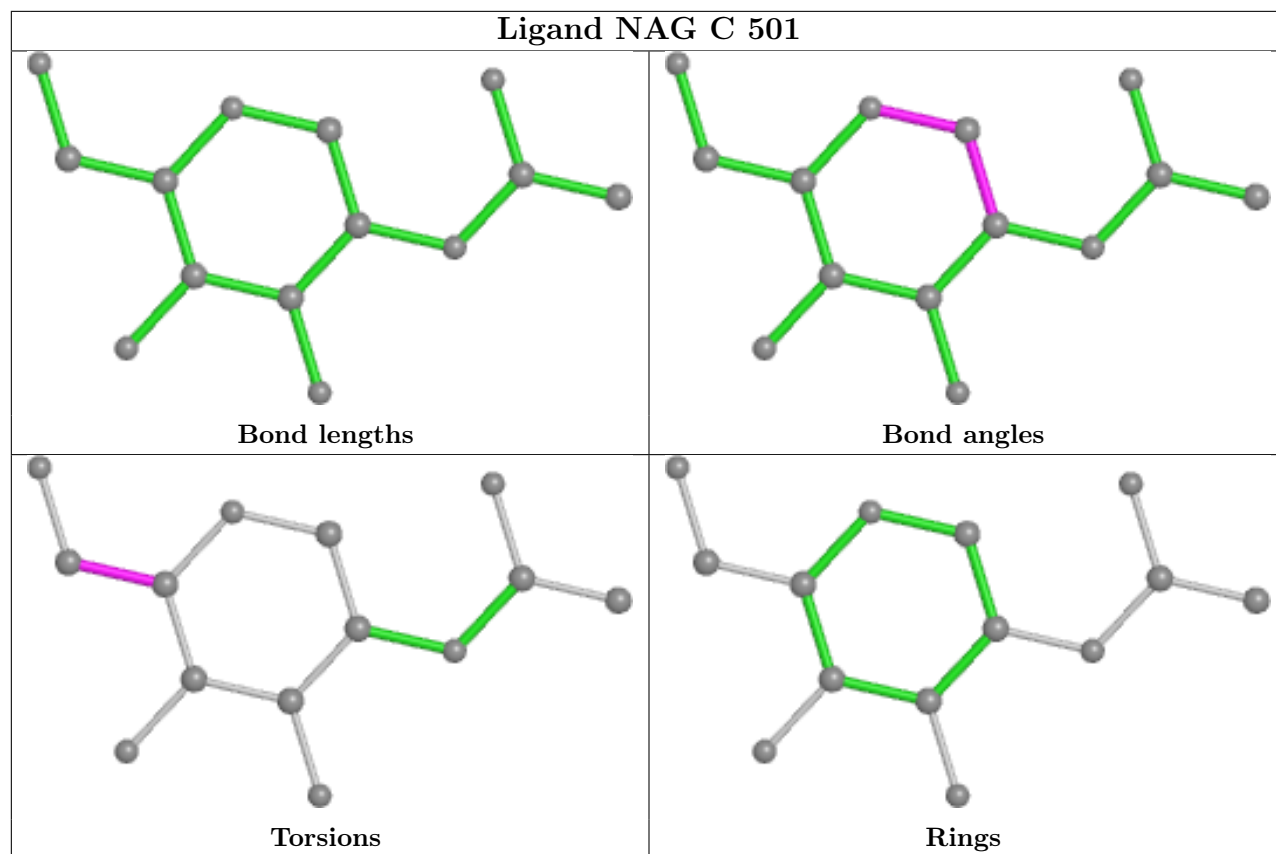


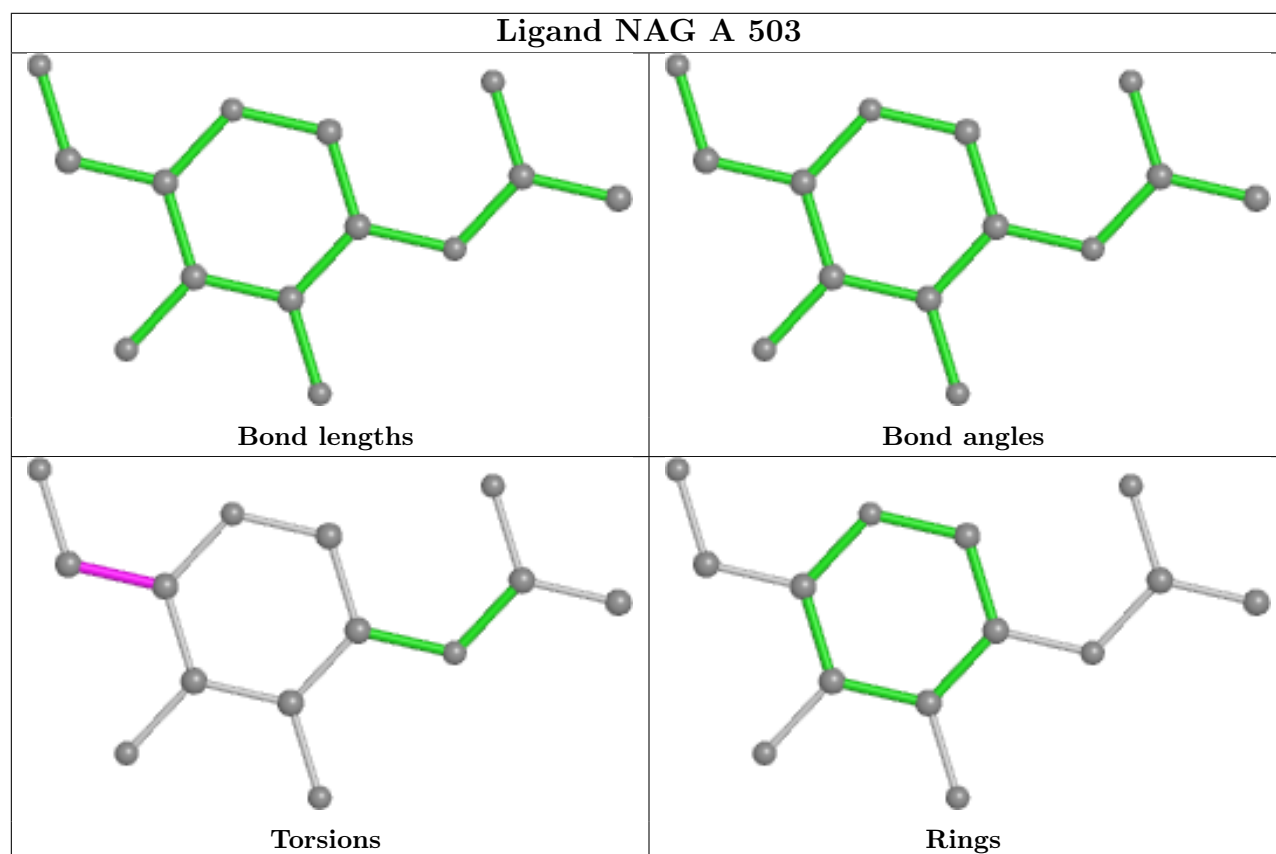
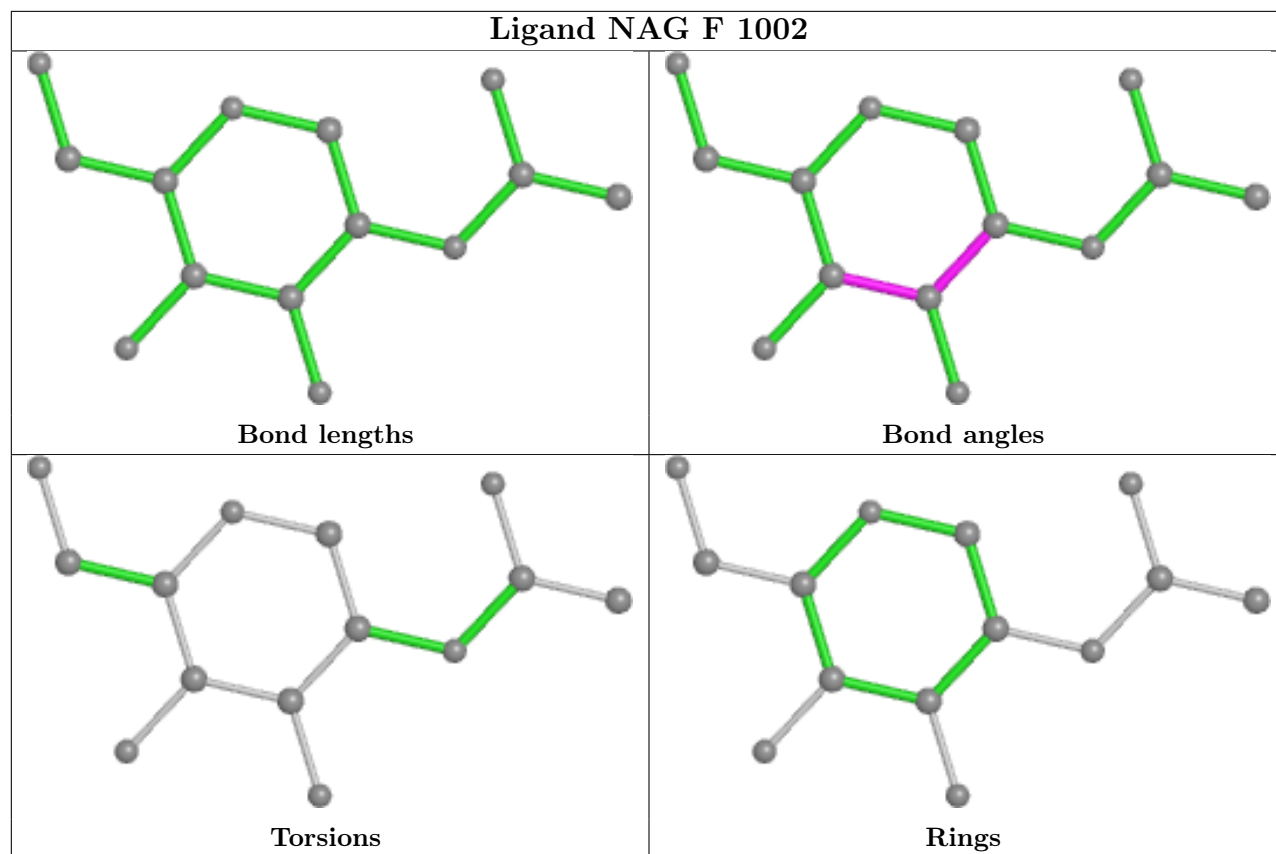




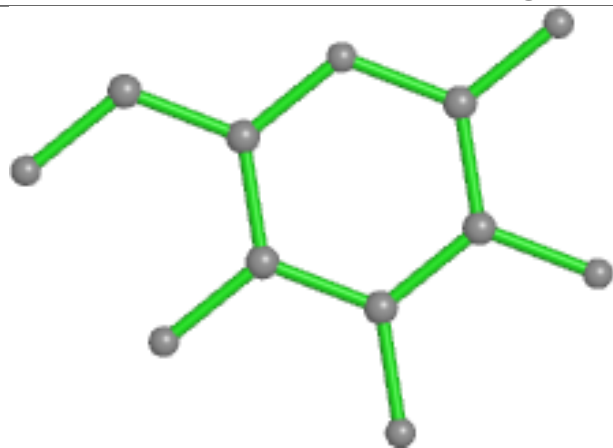




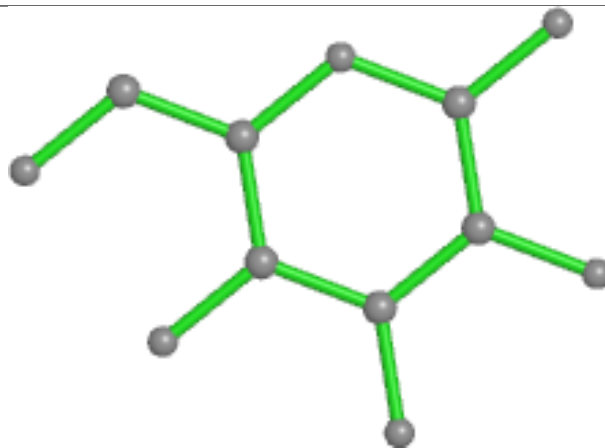




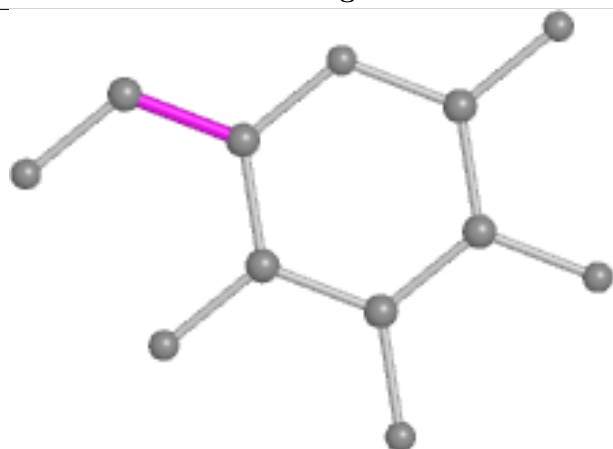
Ligand GLC I 506



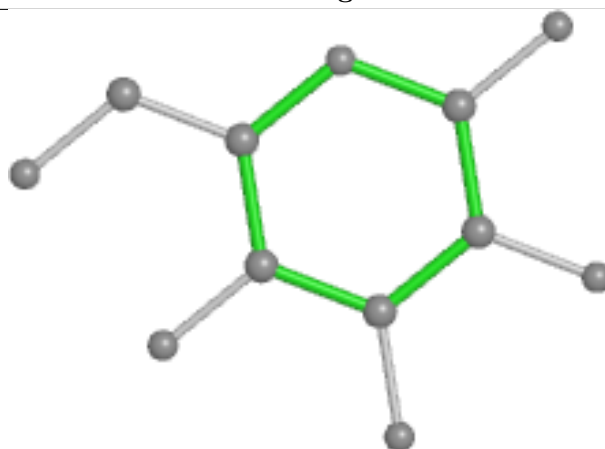
Bond lengths



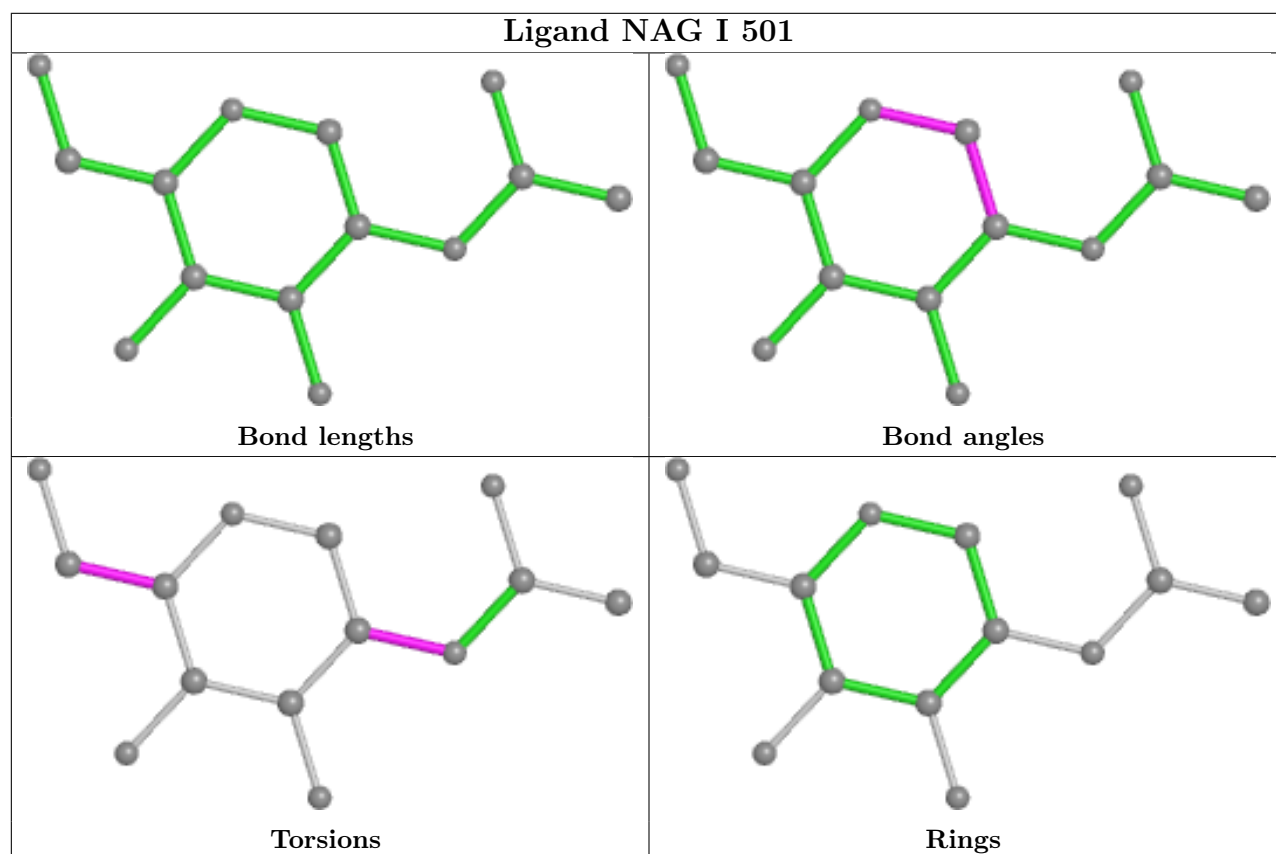
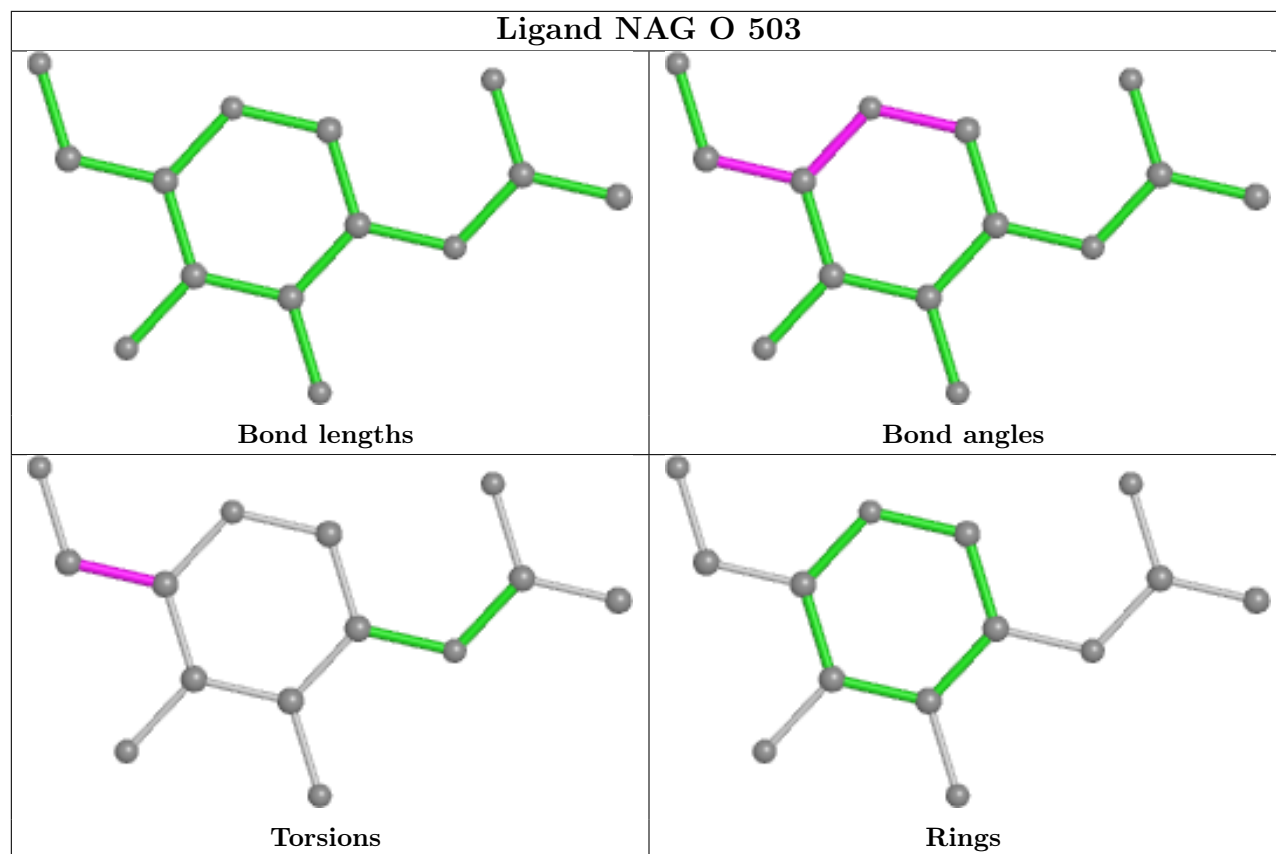
Bond angles

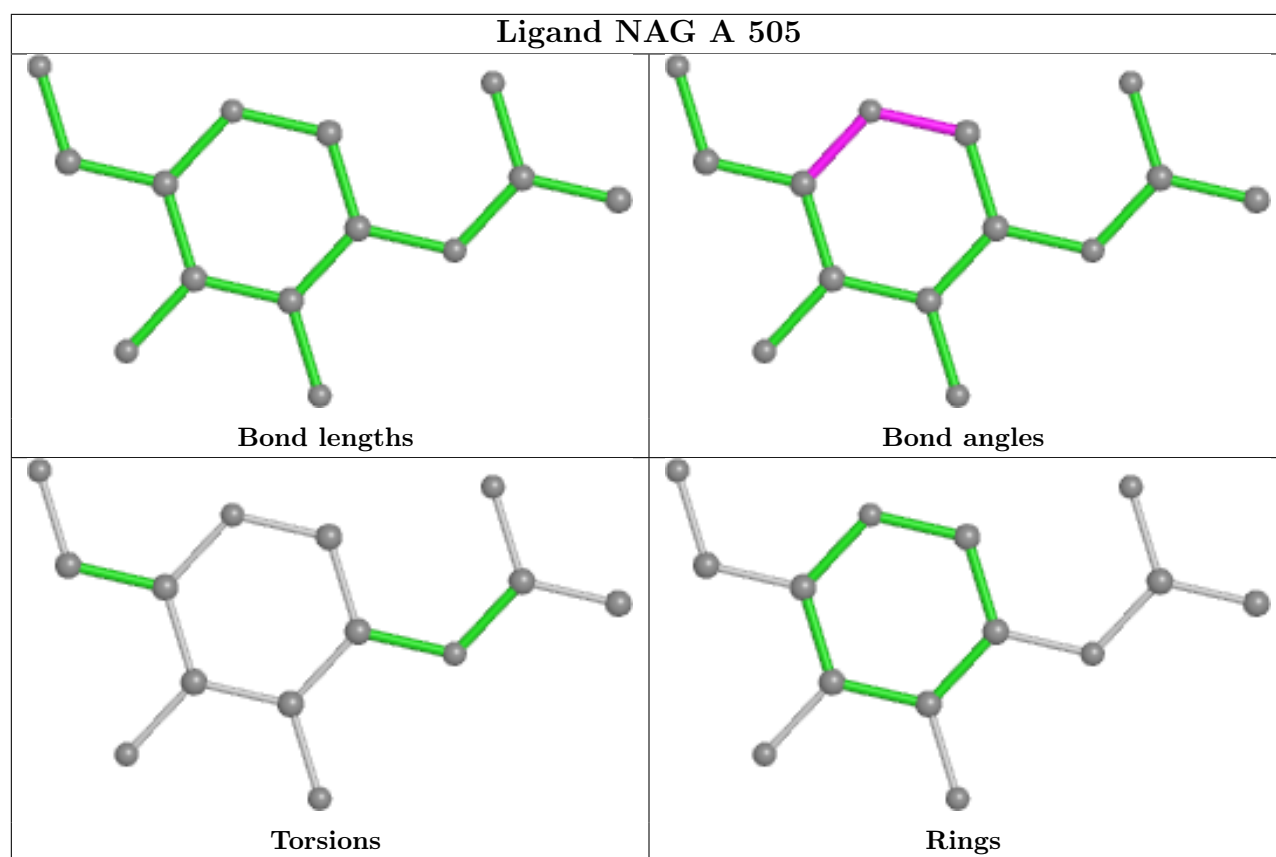


Torsions

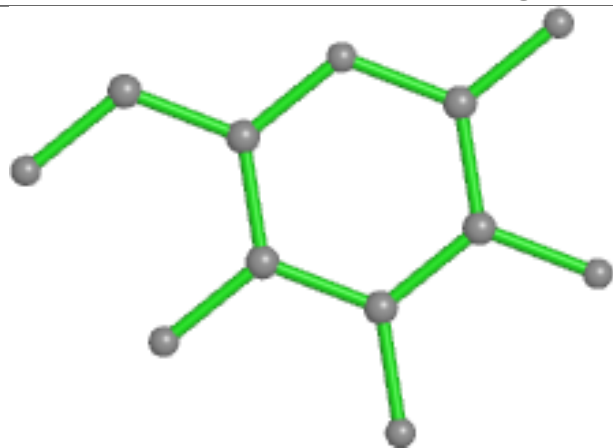


Rings

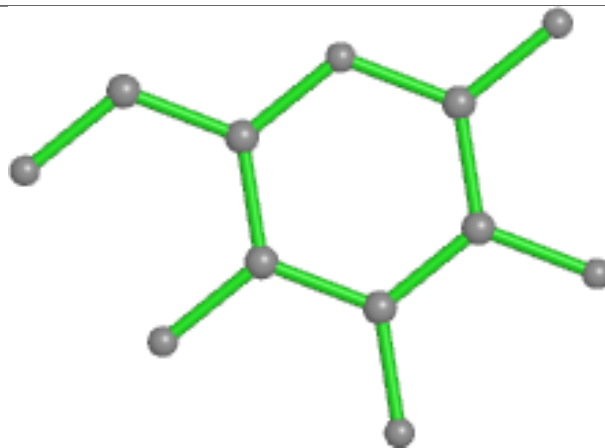




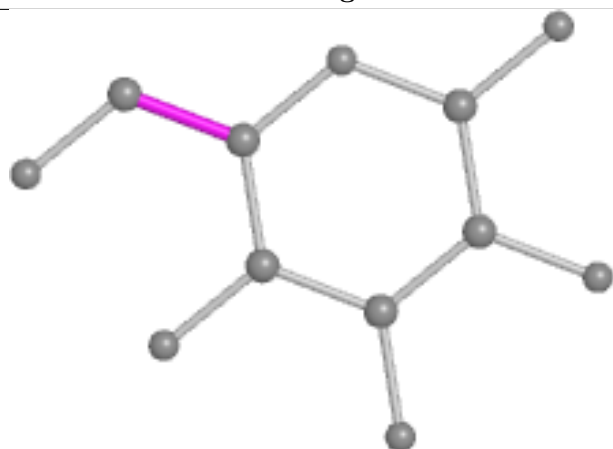
Ligand GLC E 506



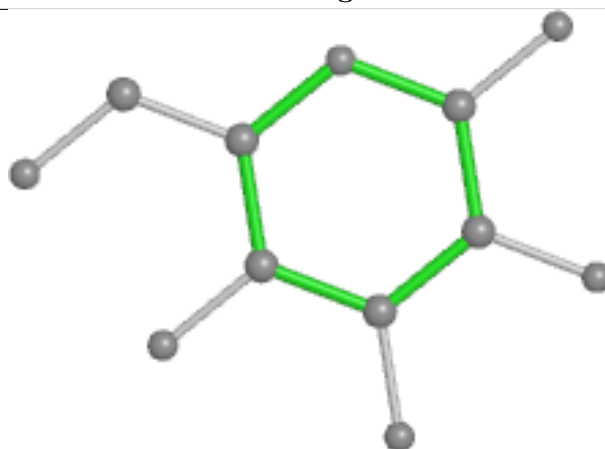
Bond lengths



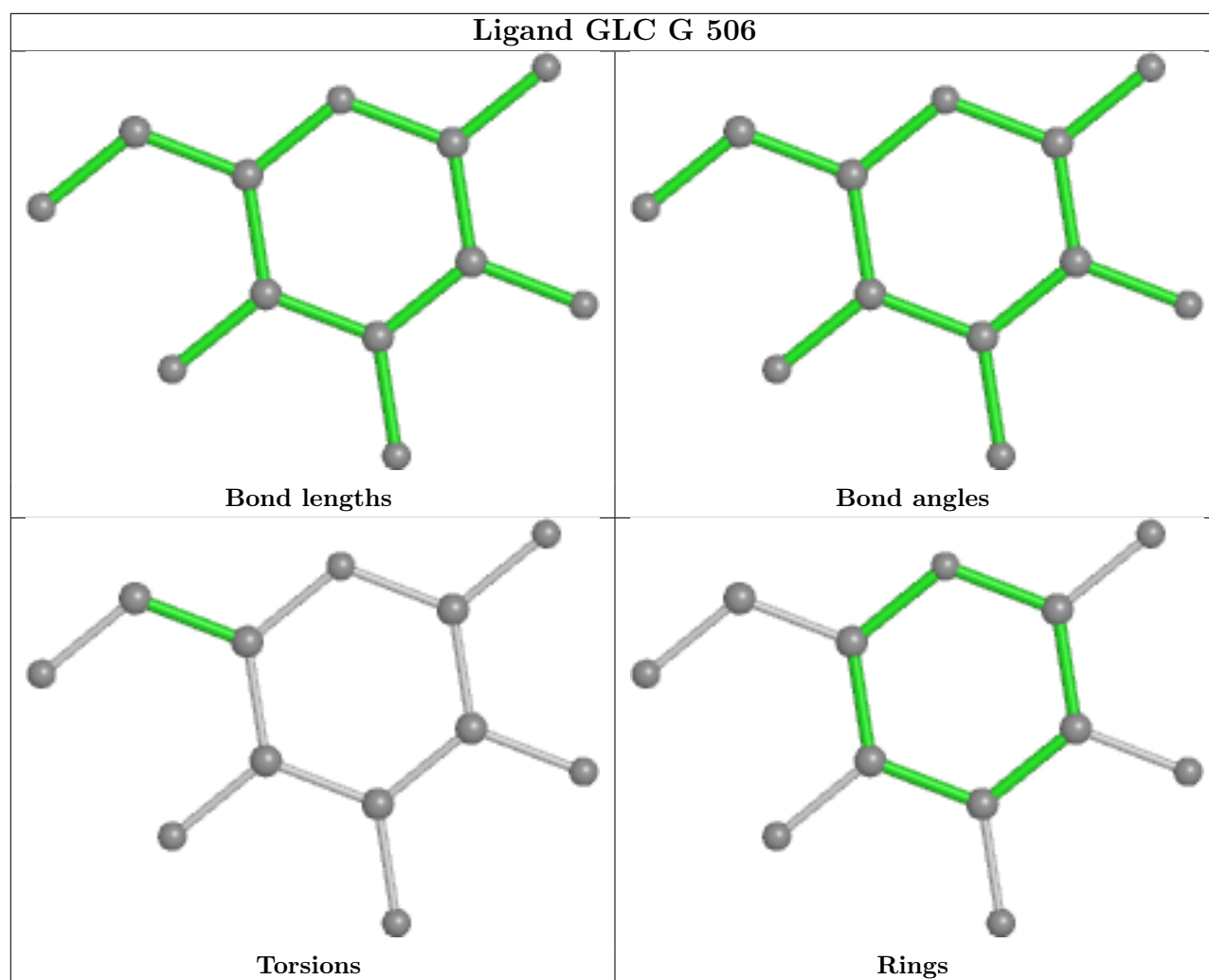
Bond angles

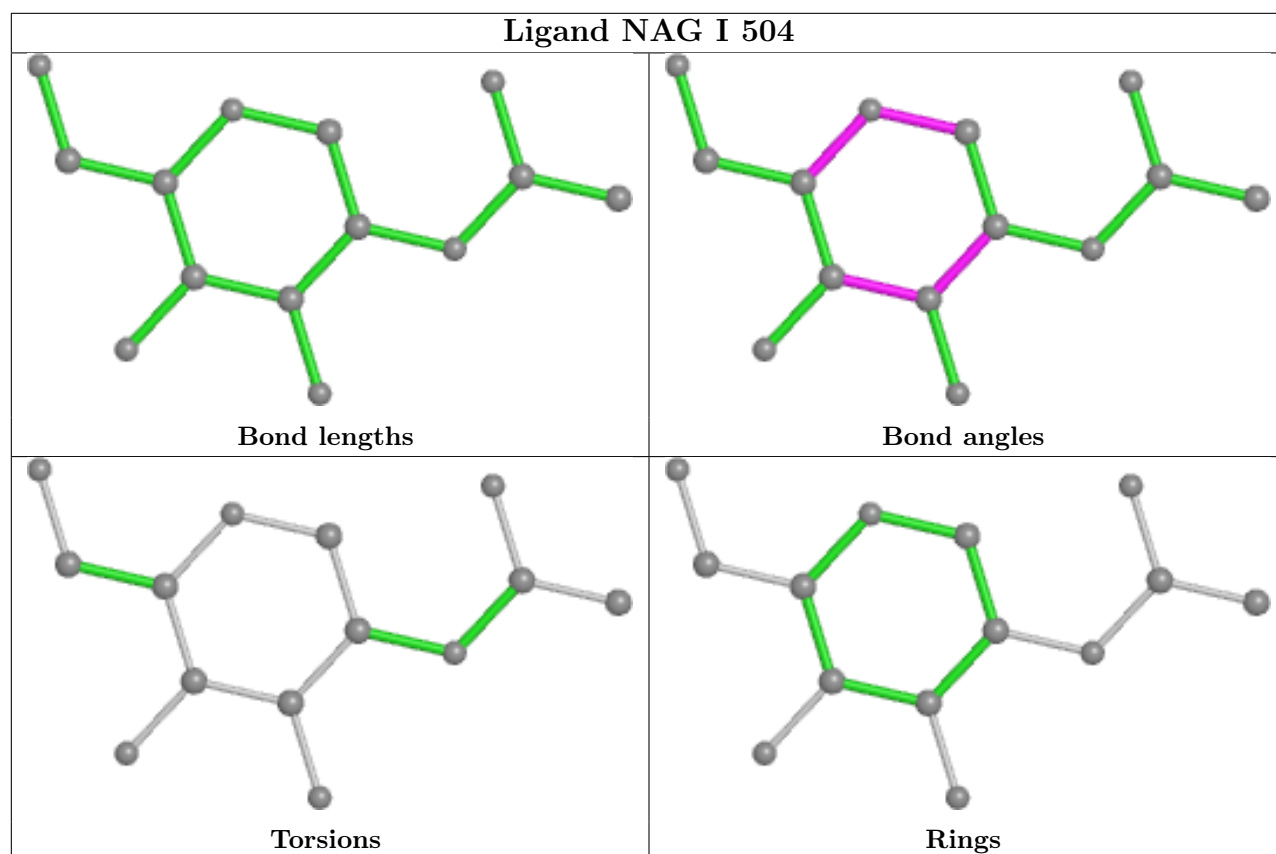
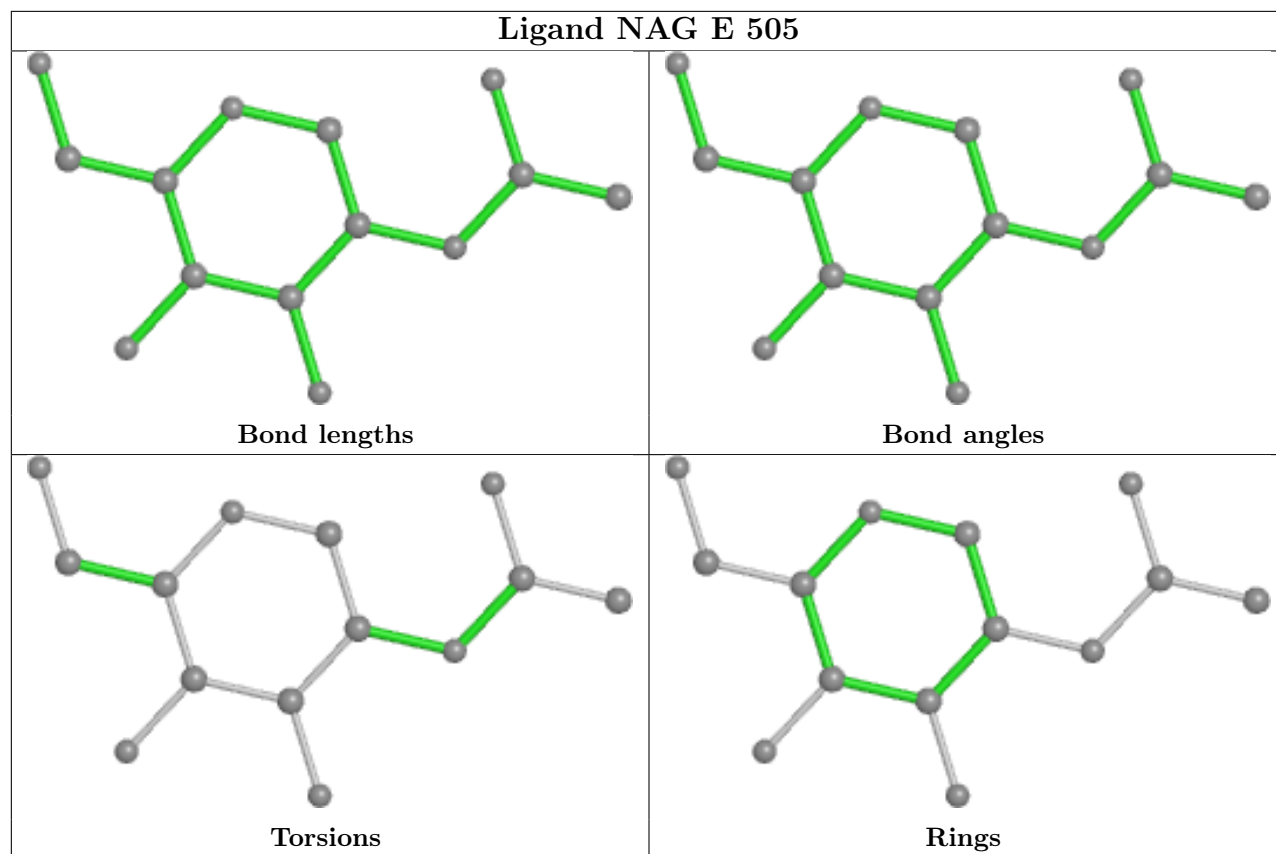


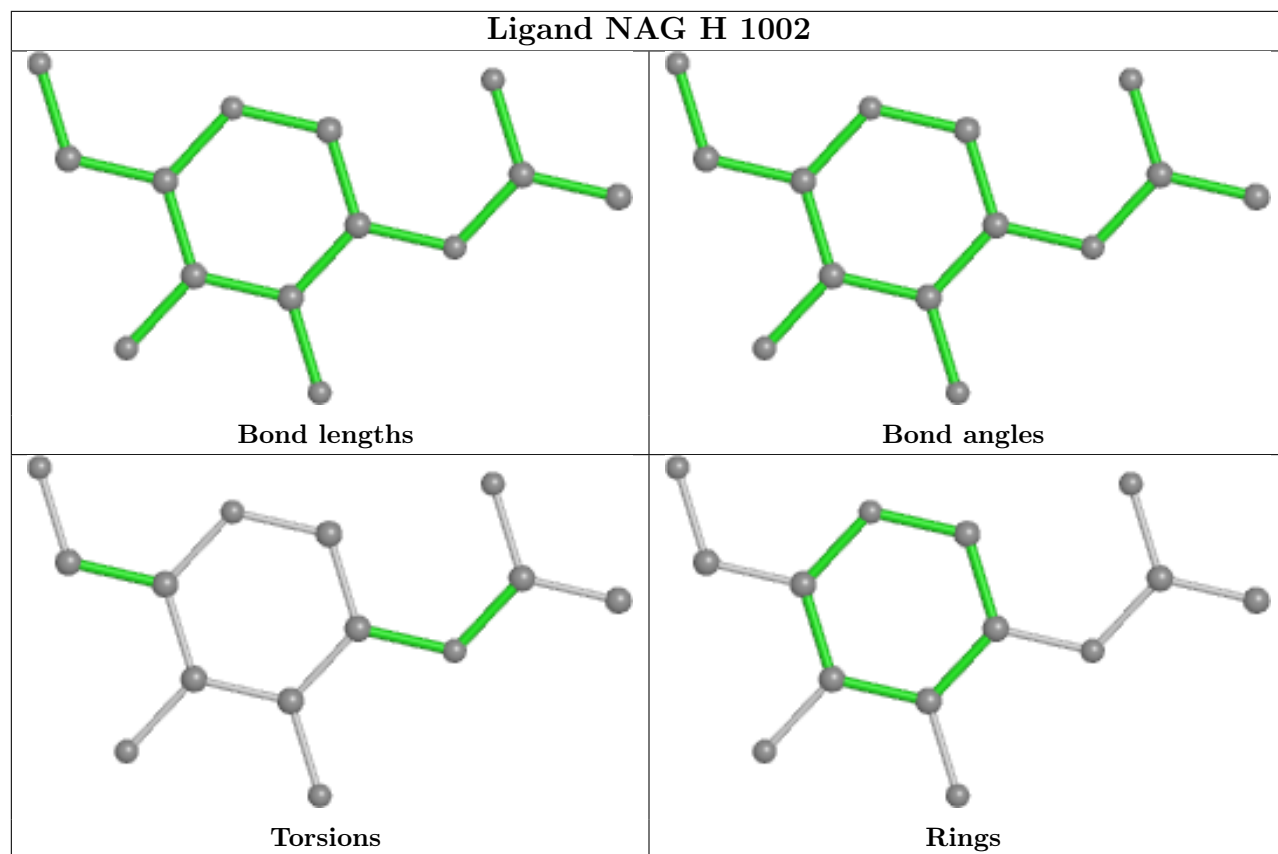
Torsions

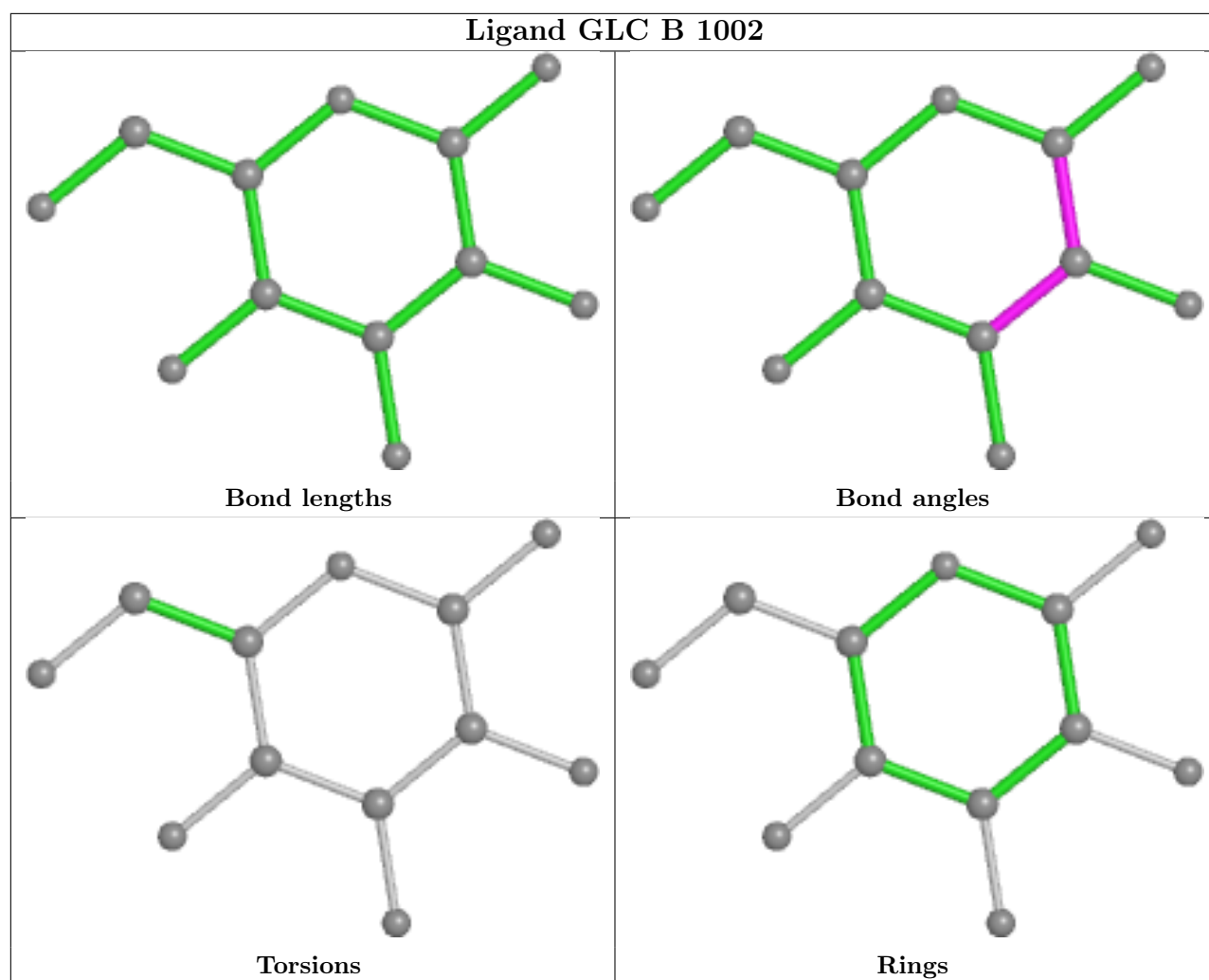


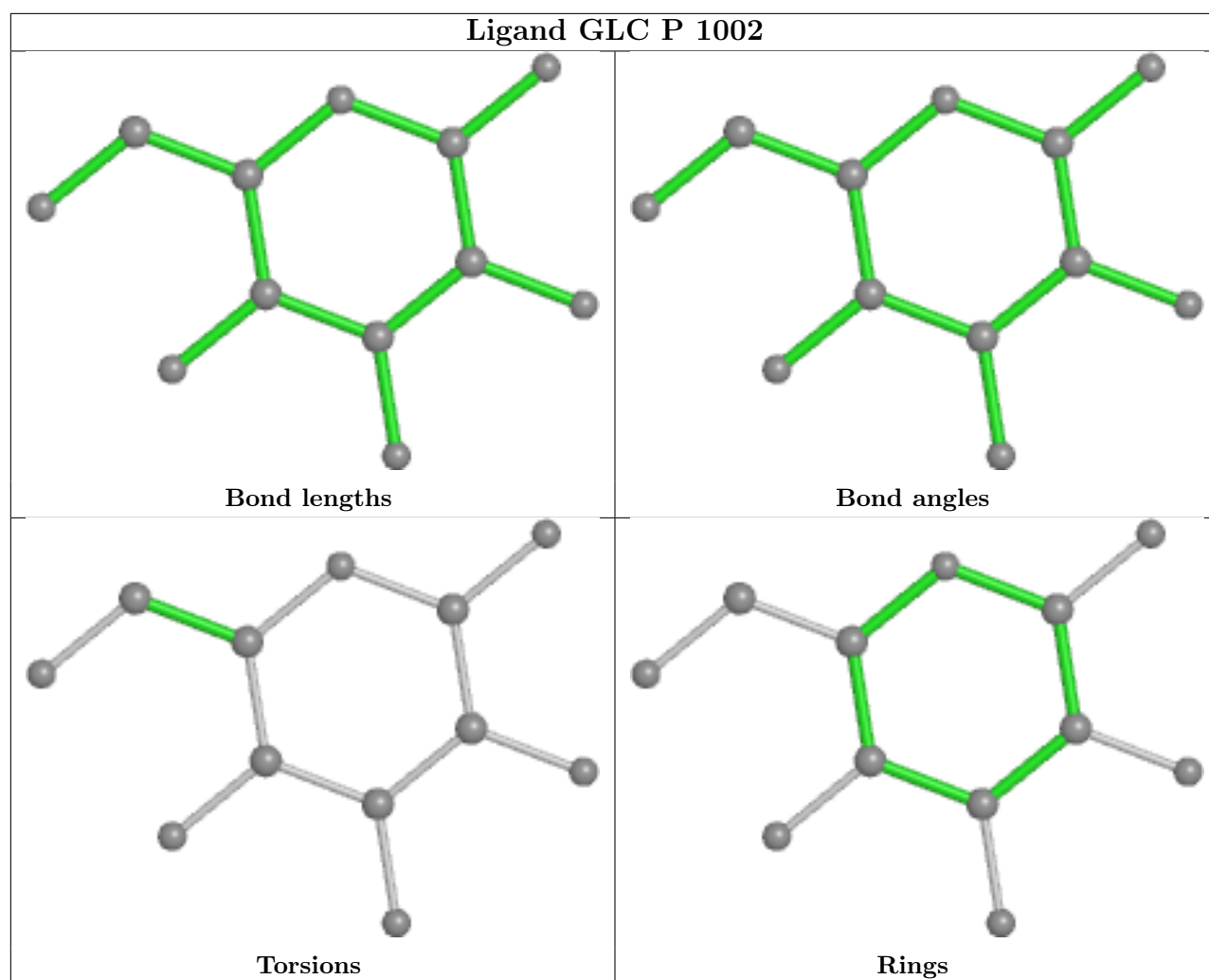
Rings

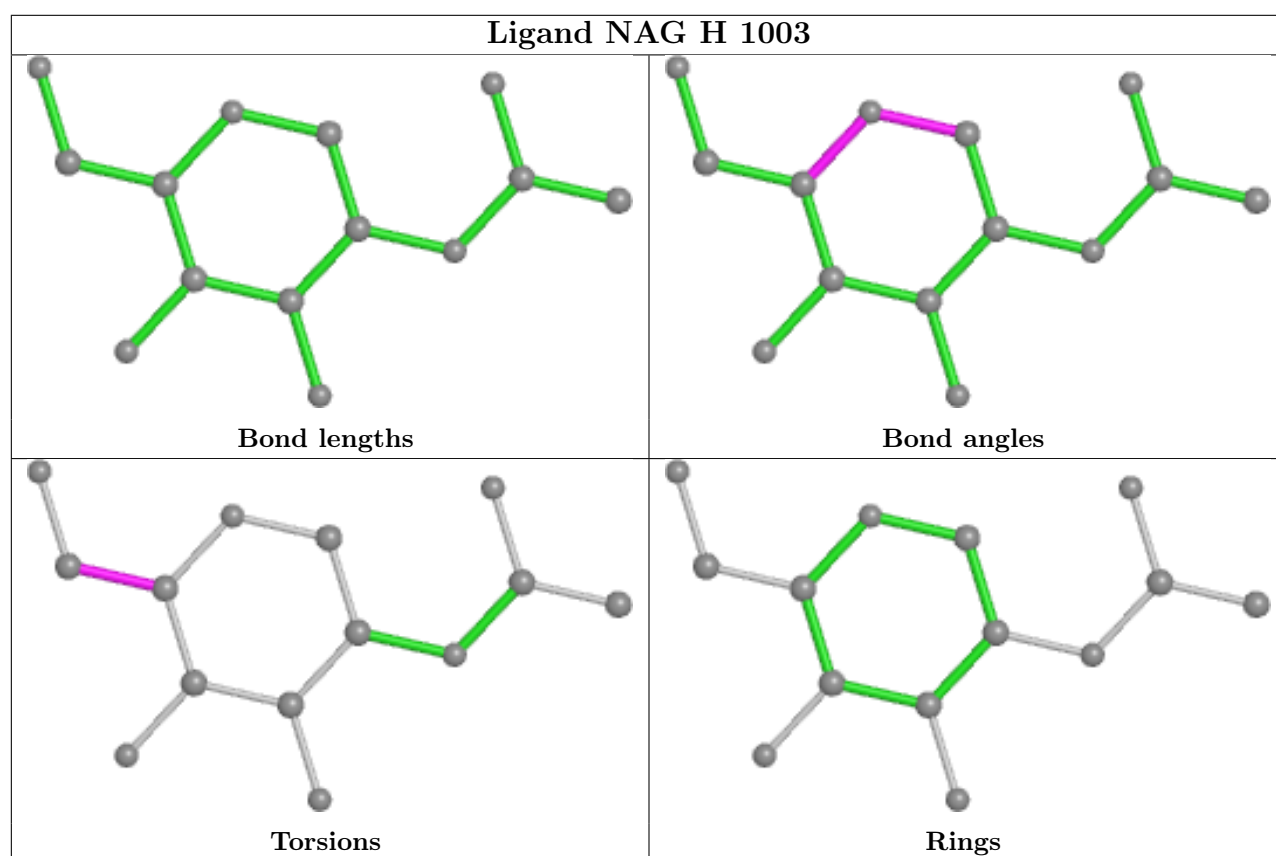
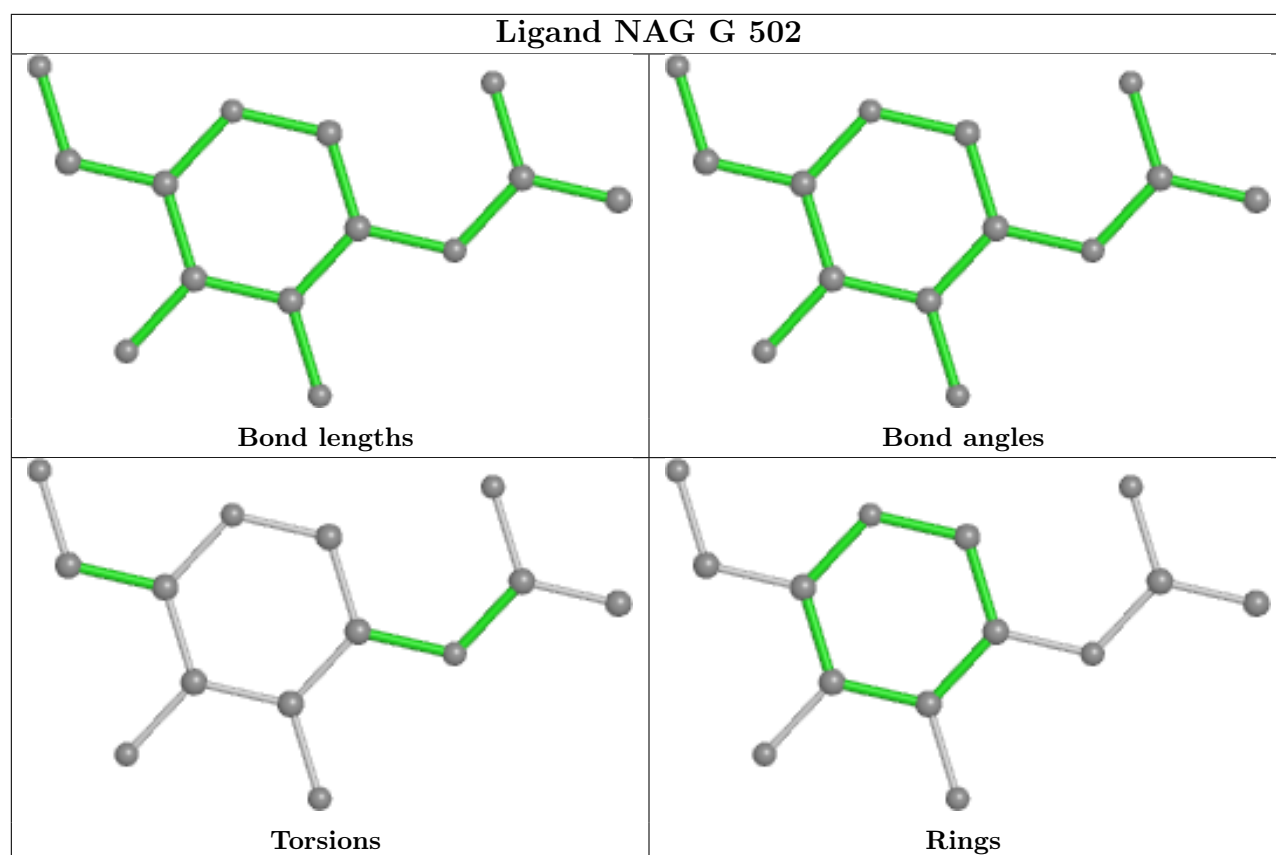


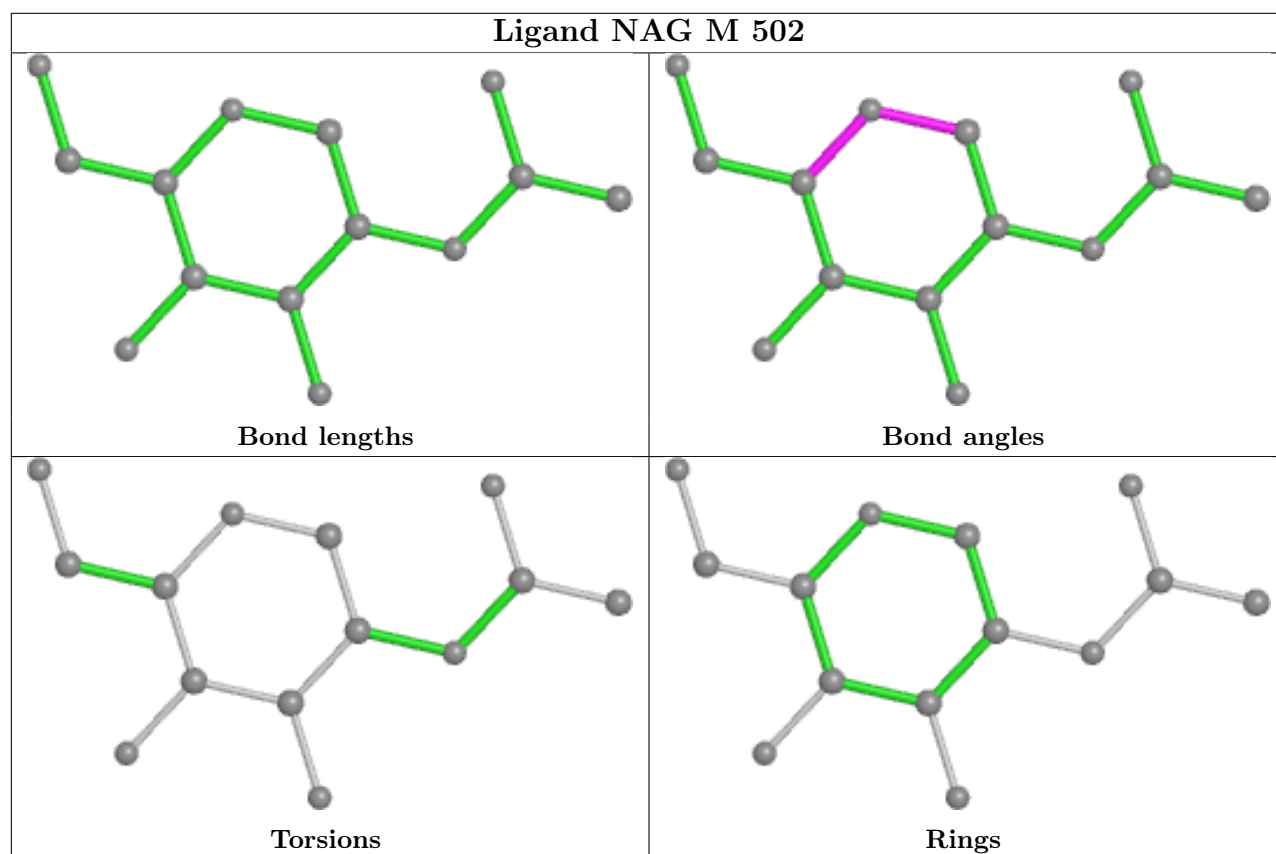
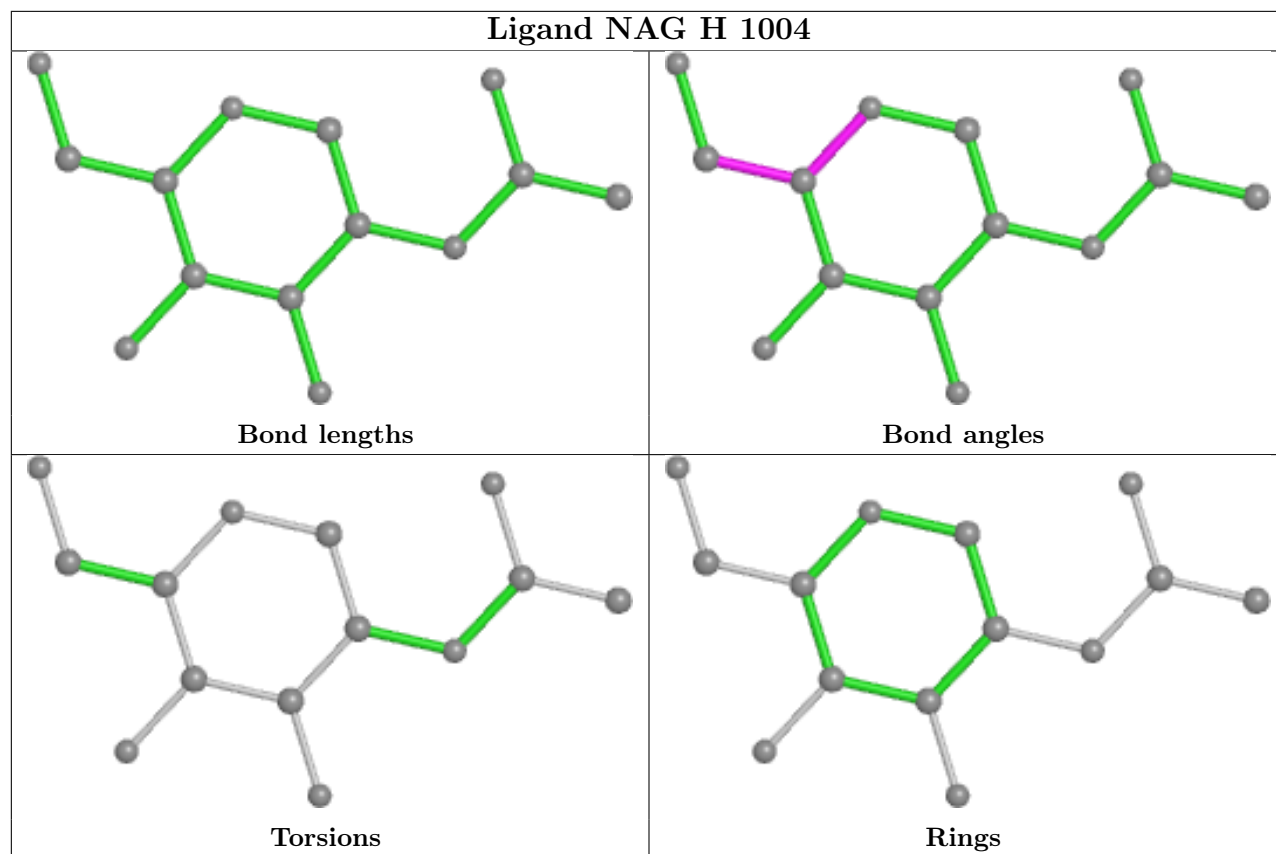




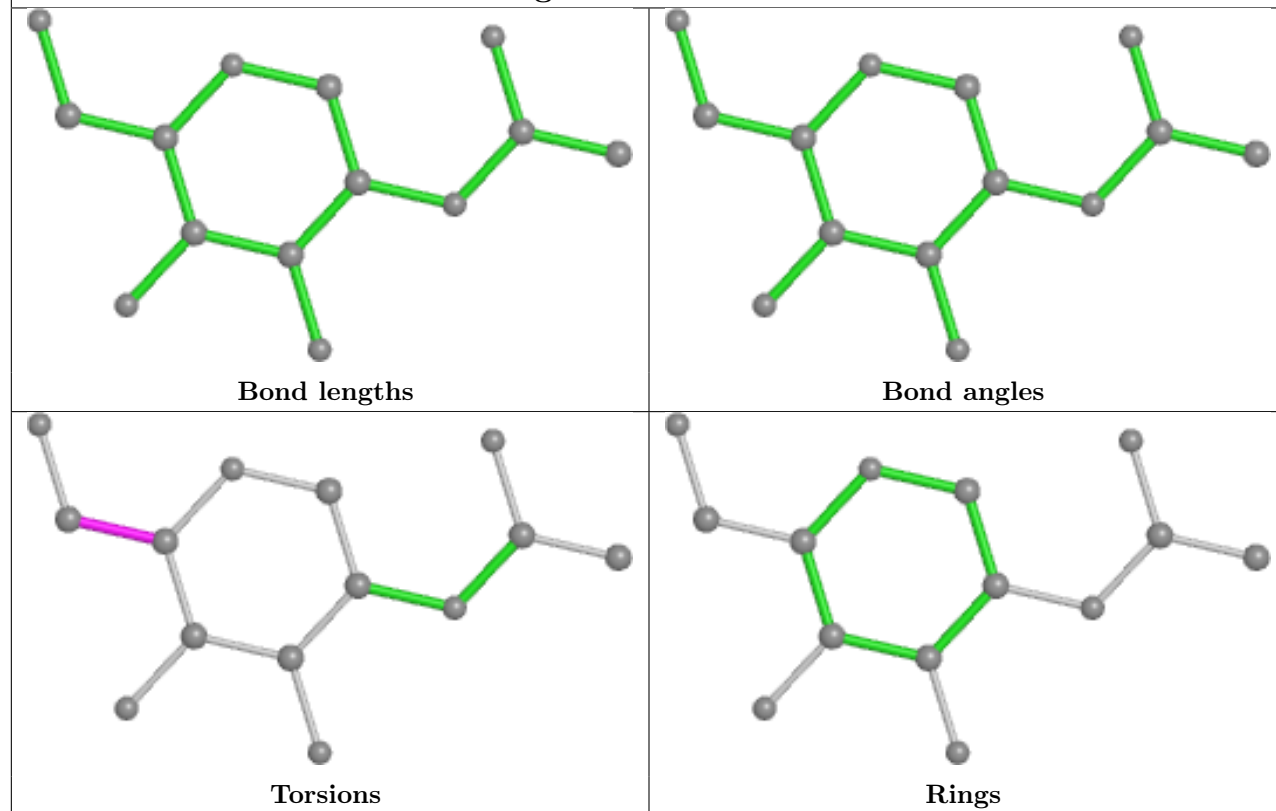




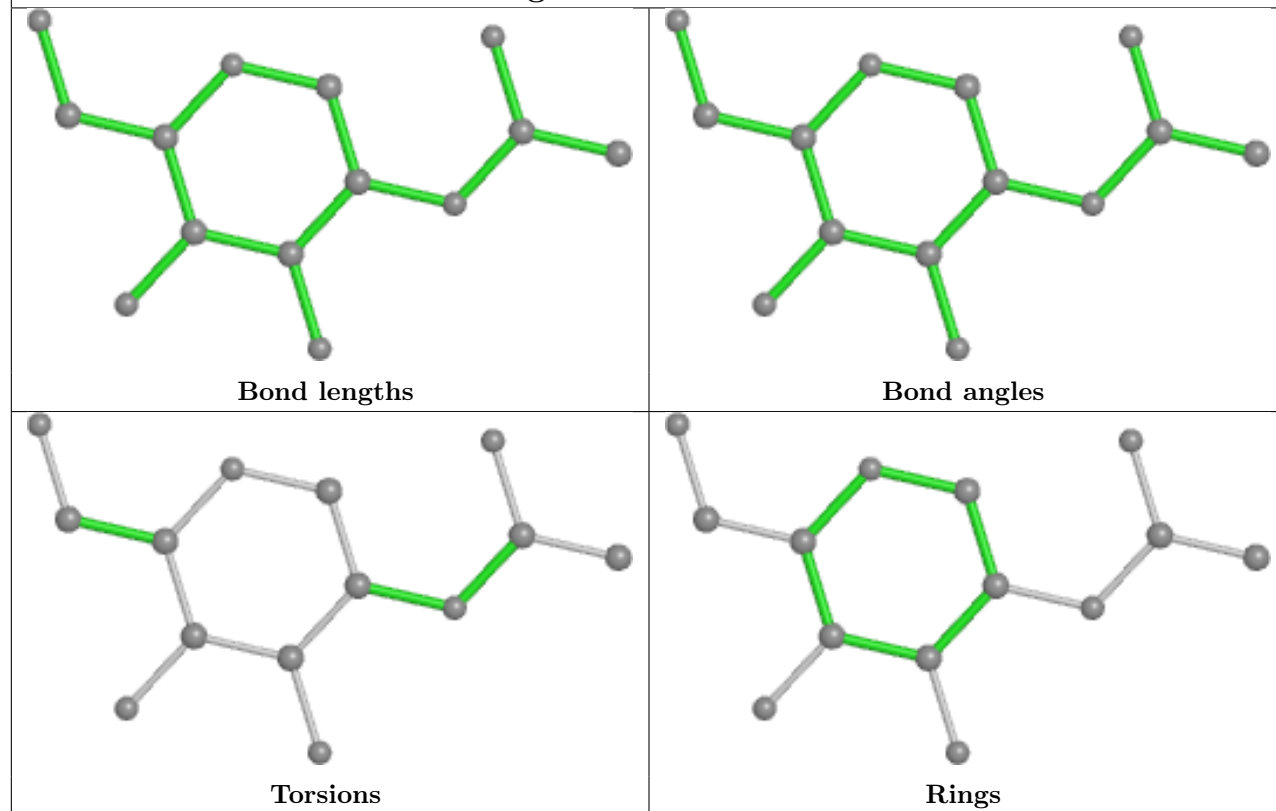


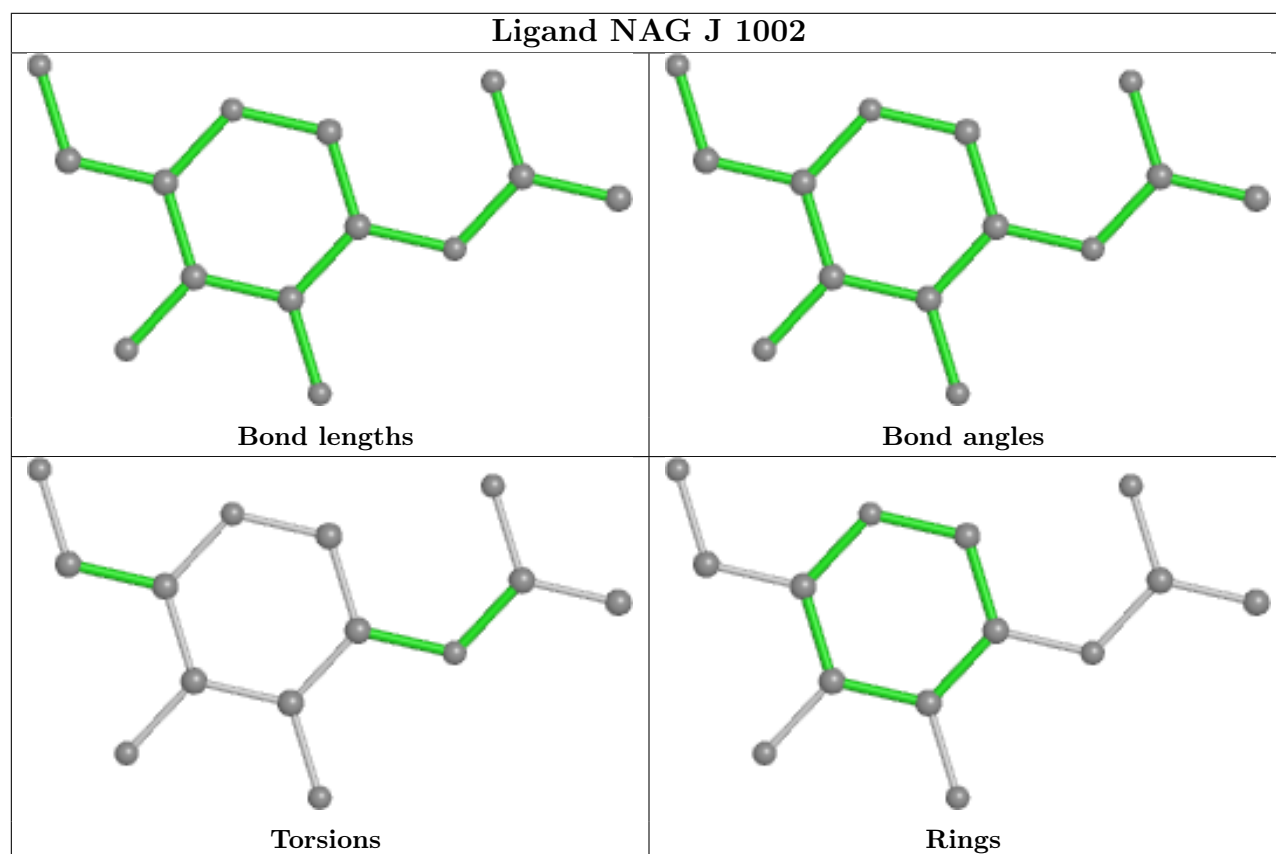
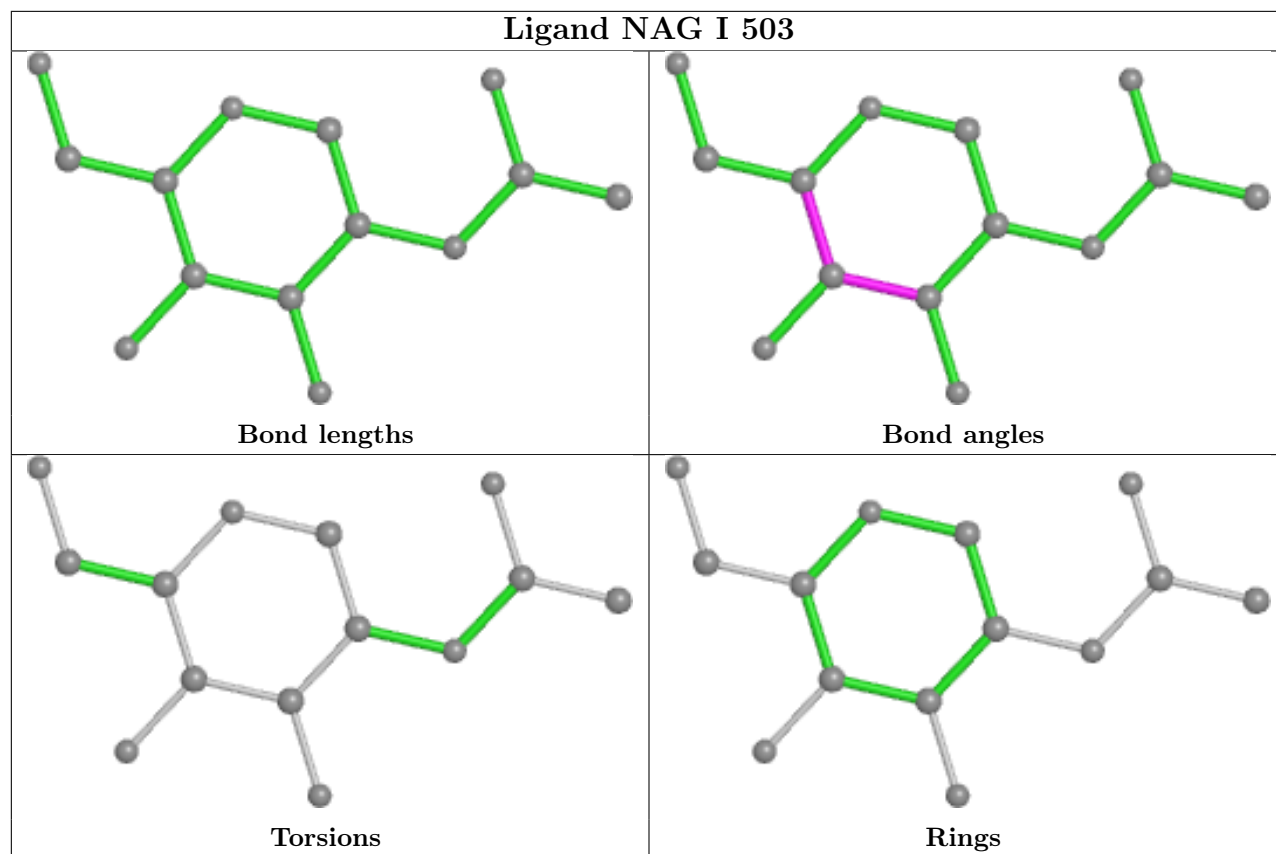


Ligand NAG I 505

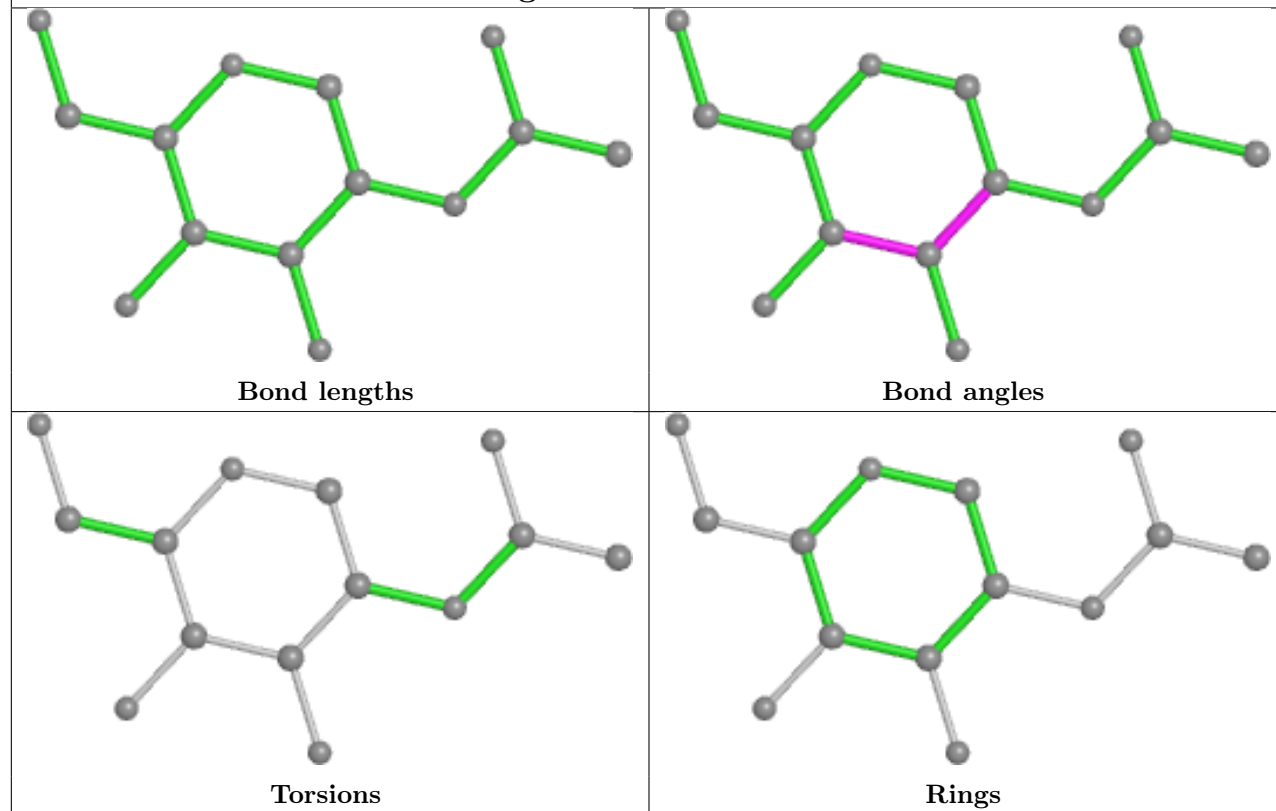


Ligand NAG A 501

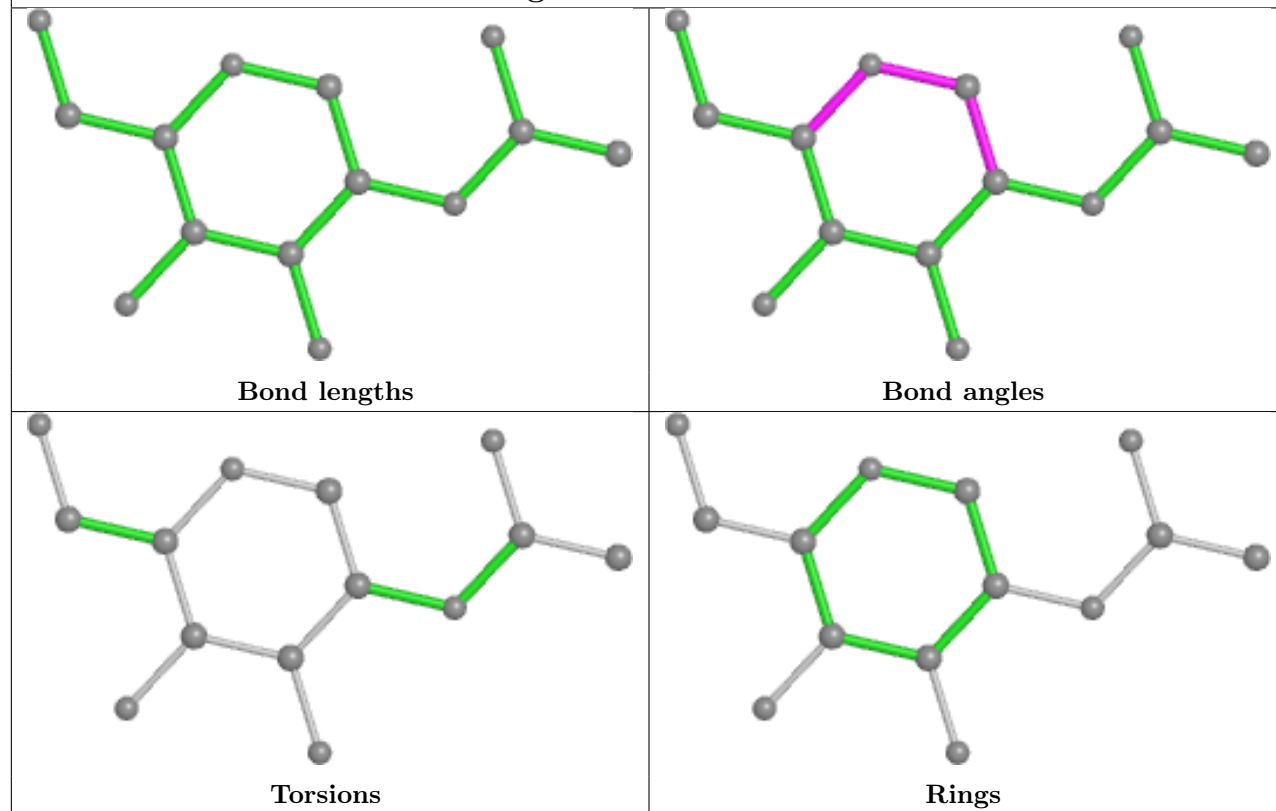


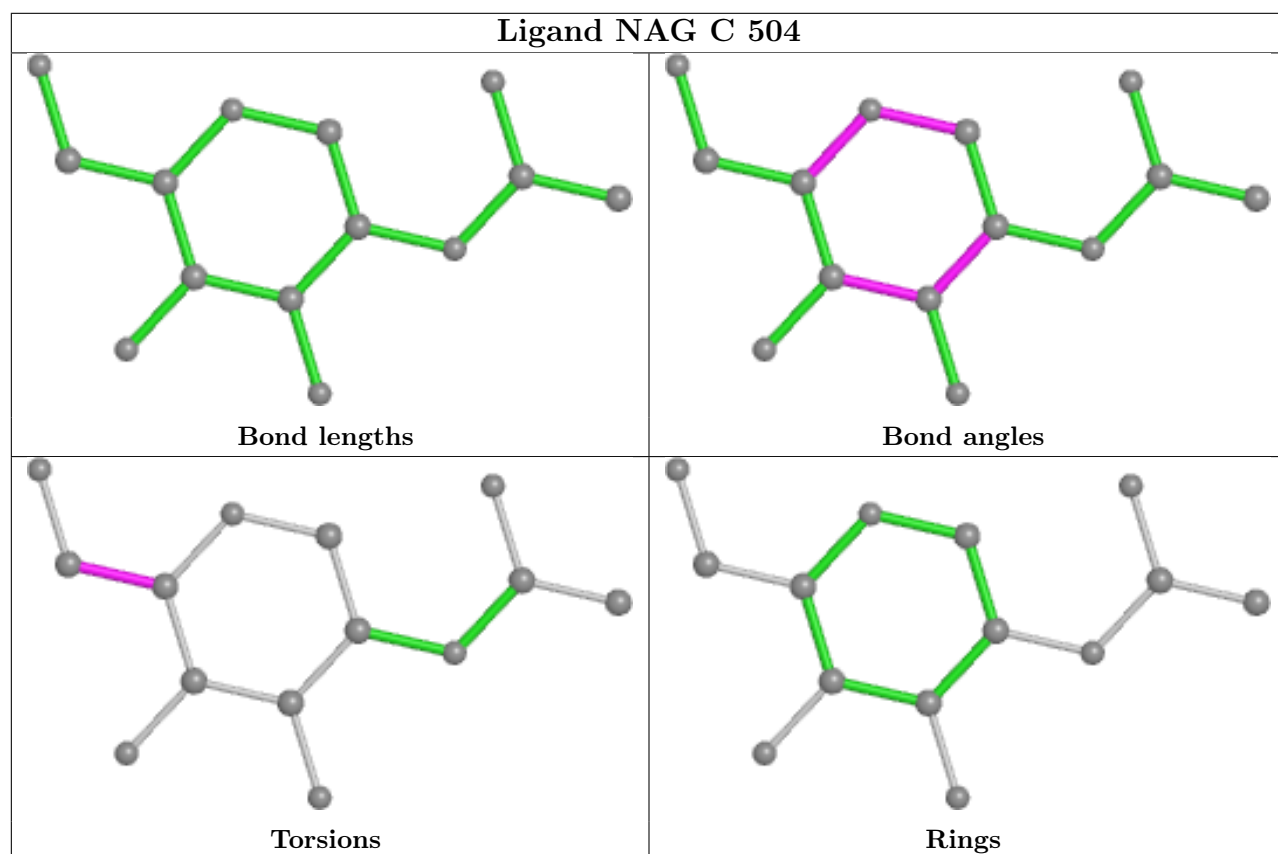
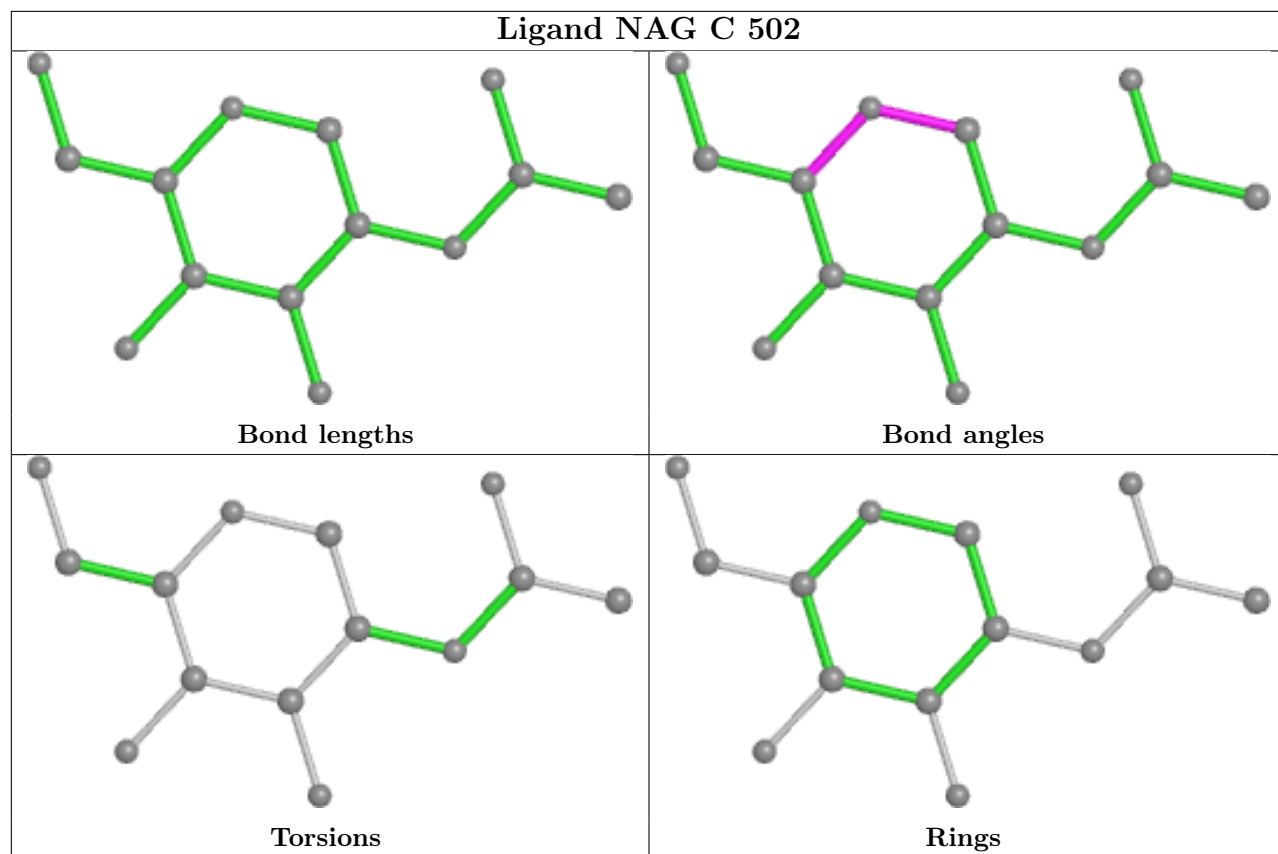


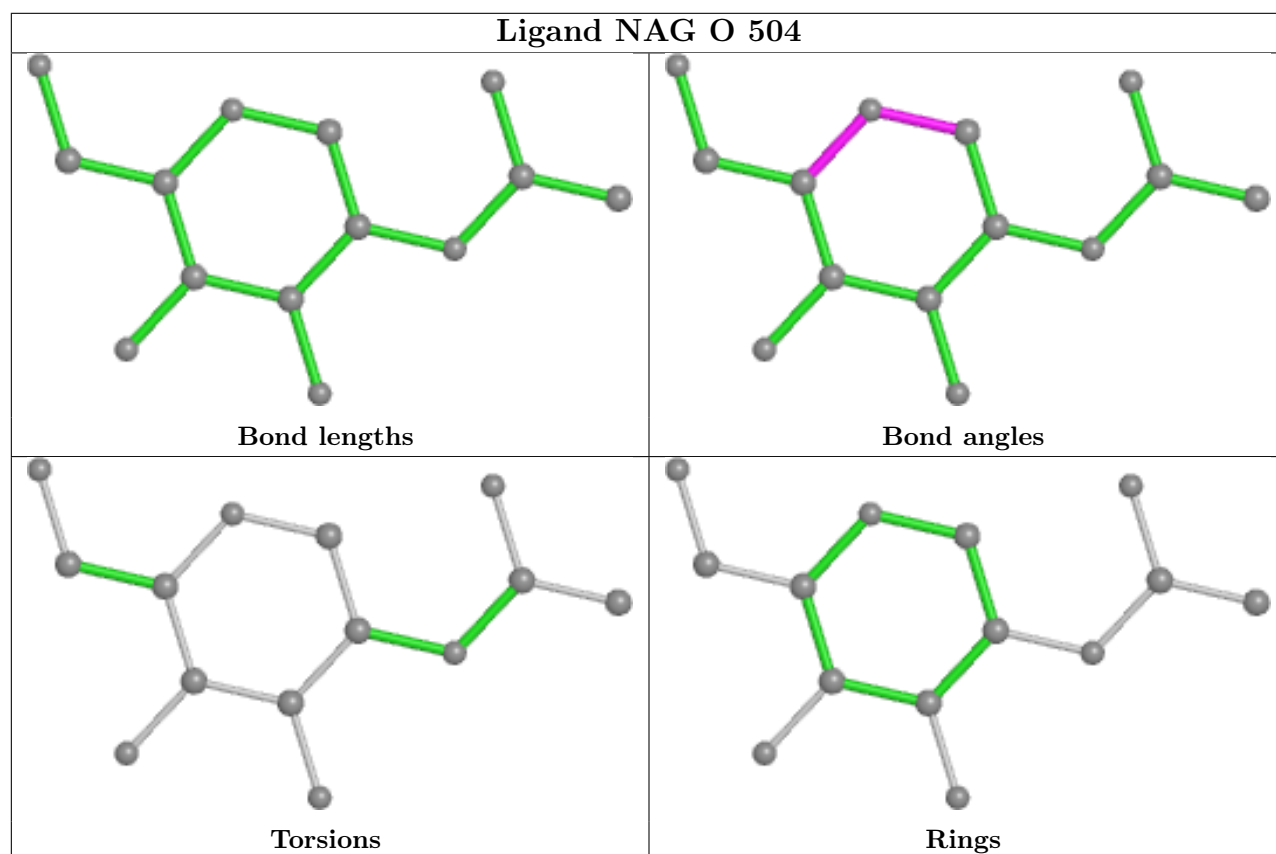
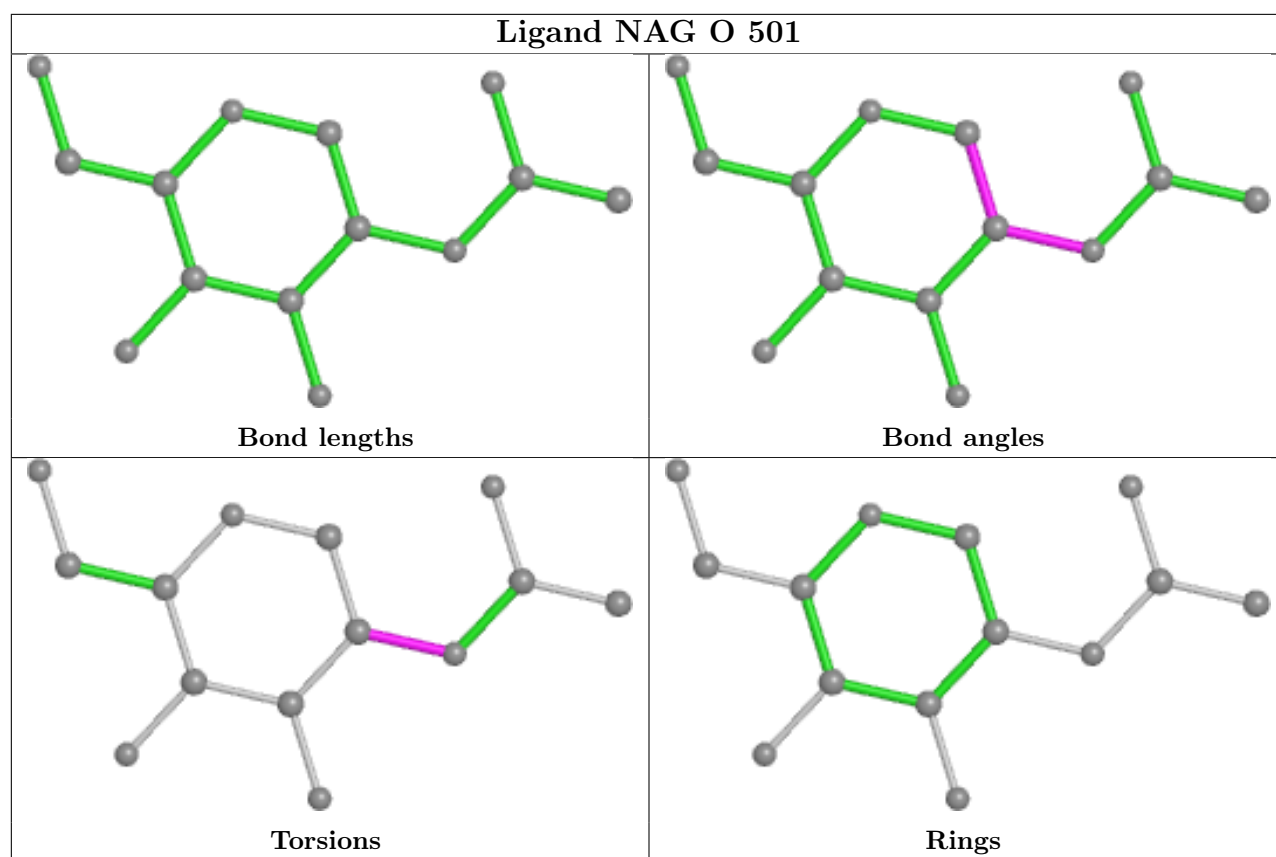
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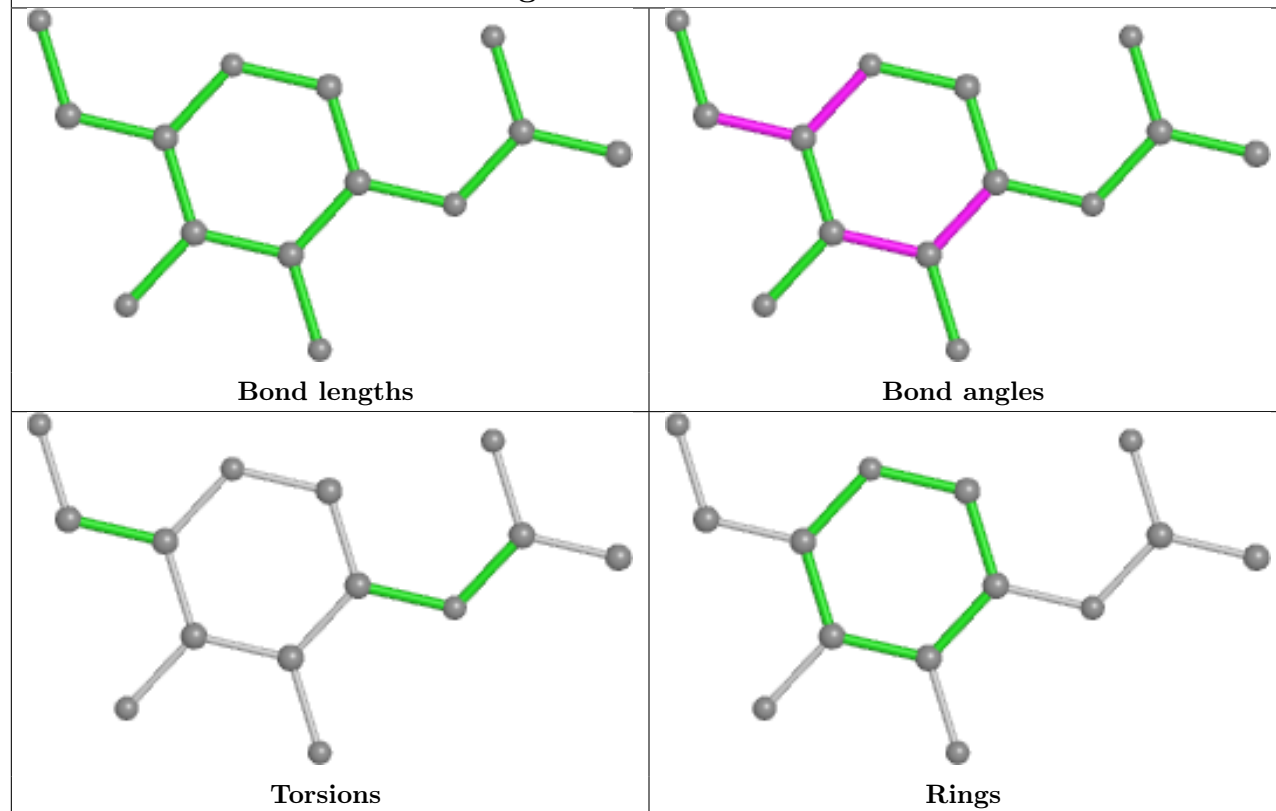
Ligand NAG G 505



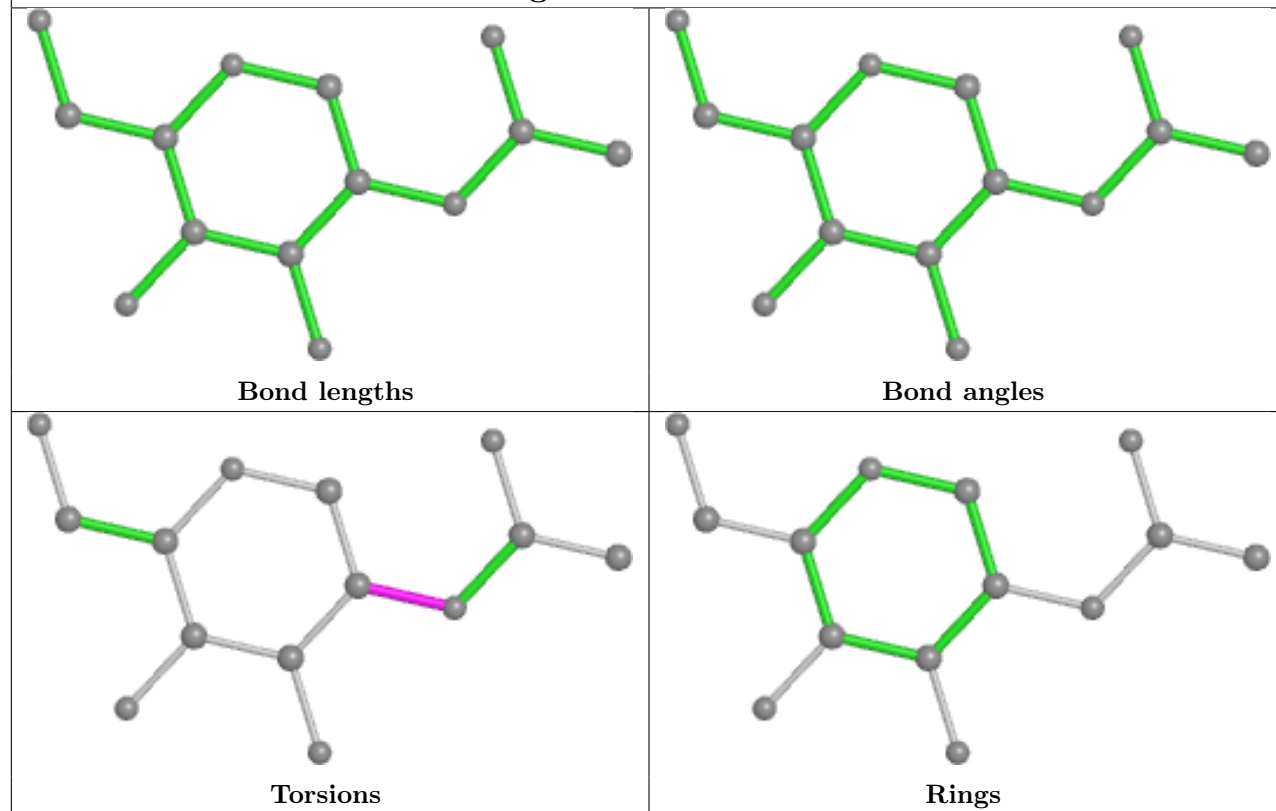




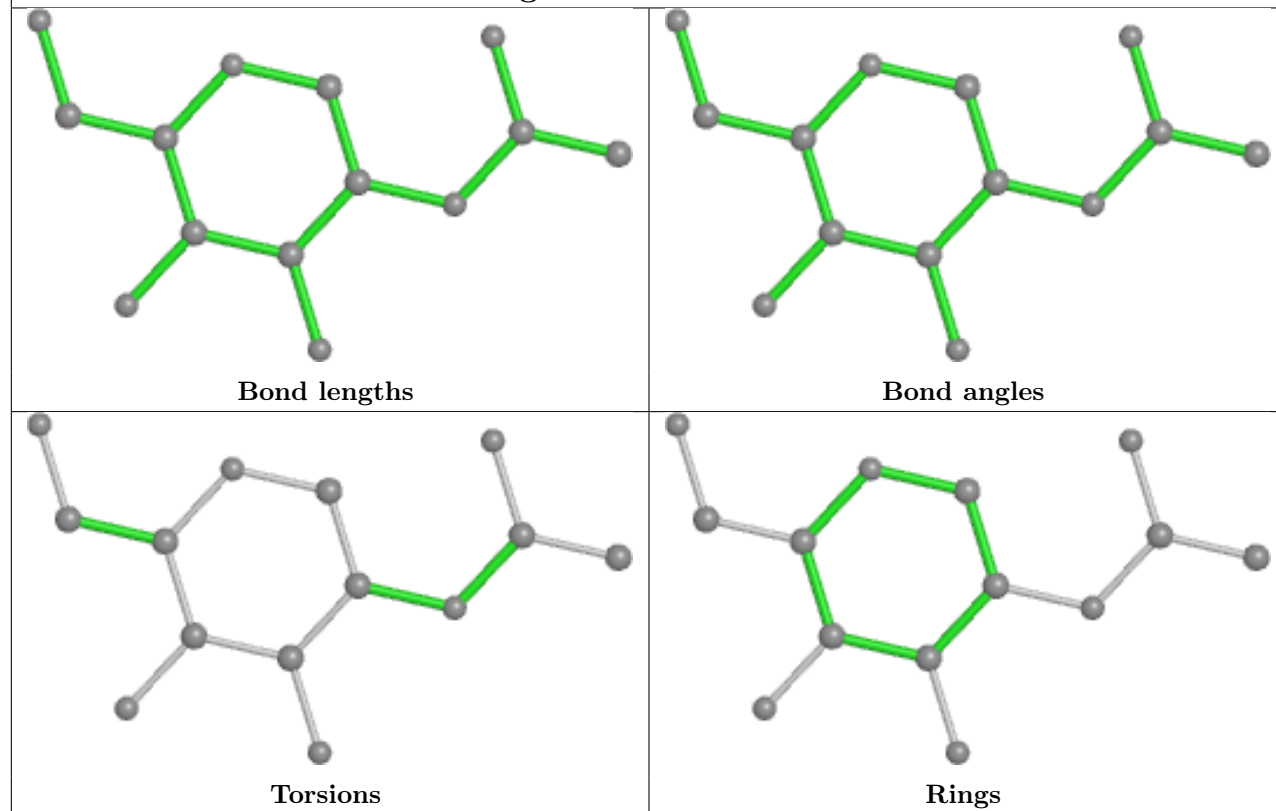
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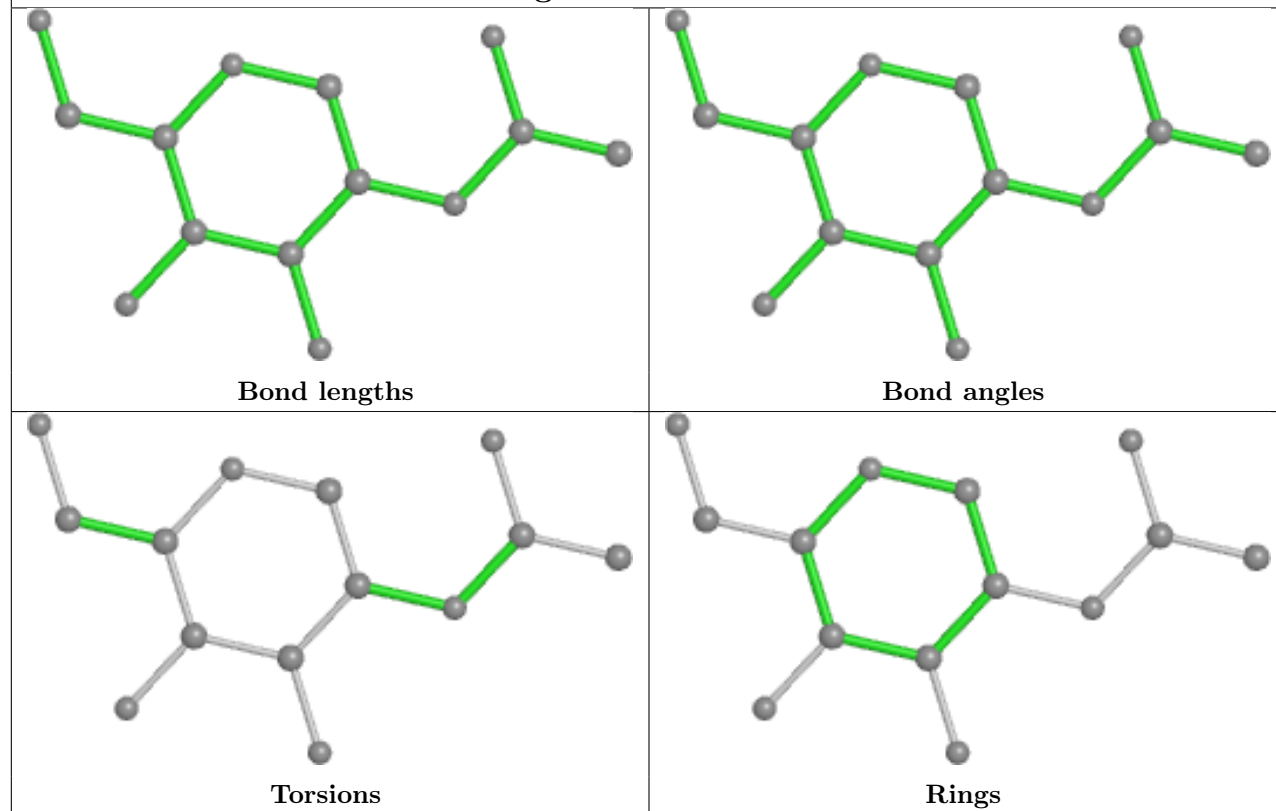
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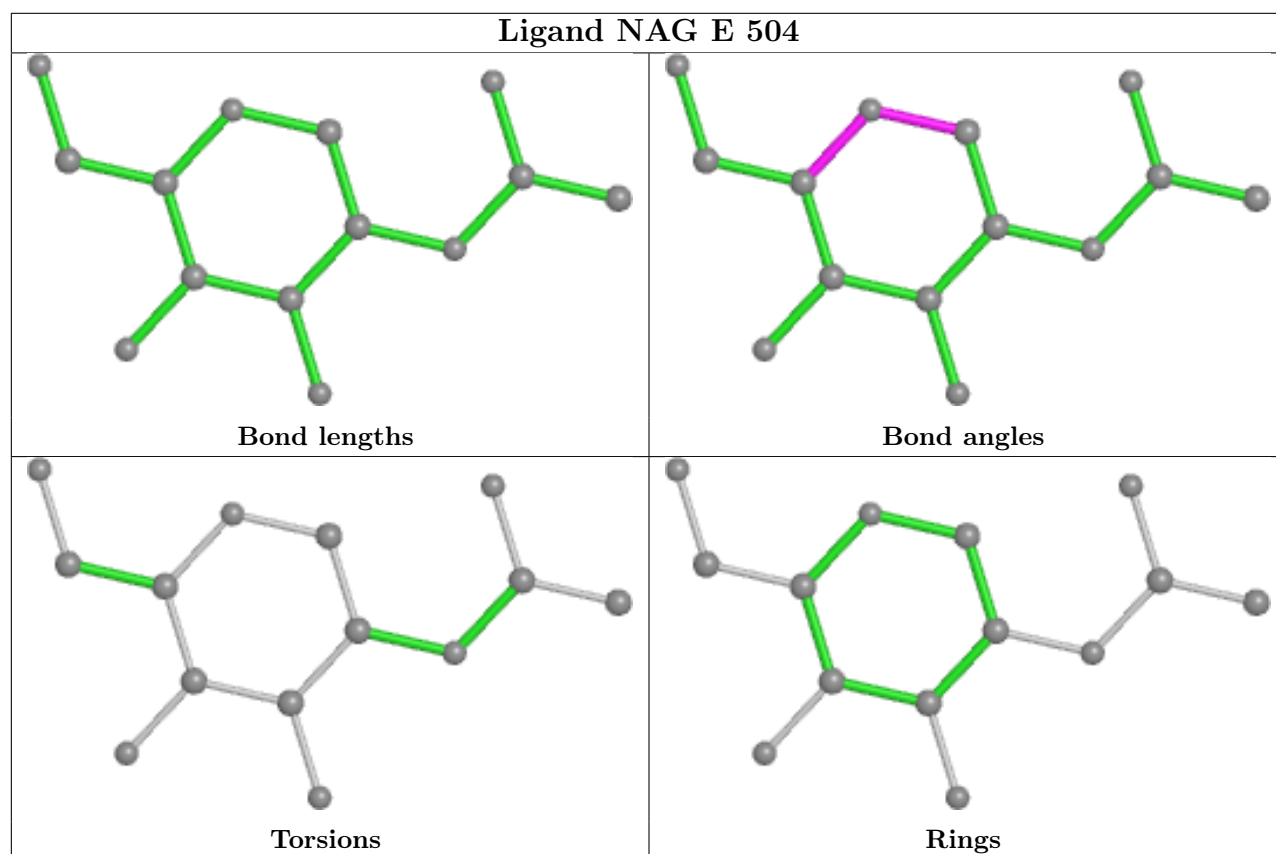
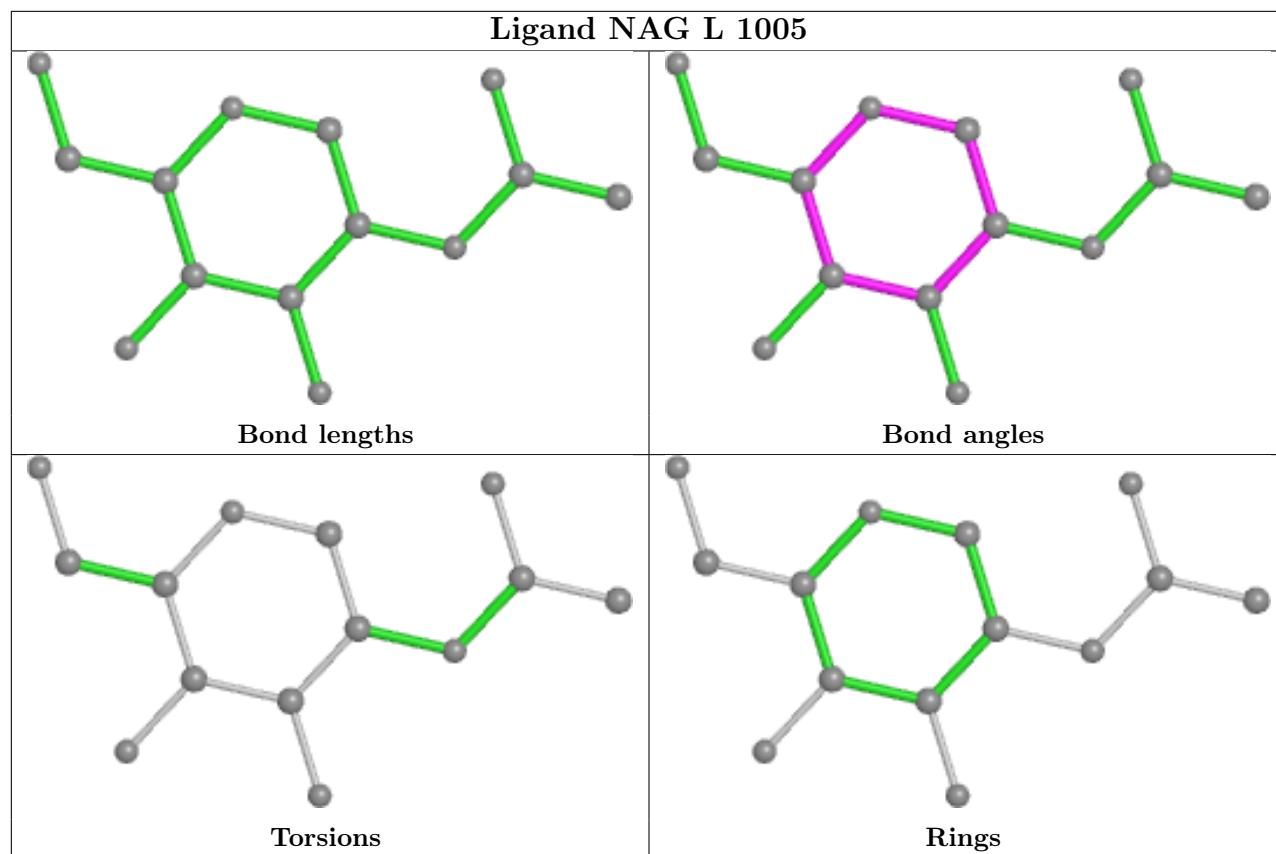


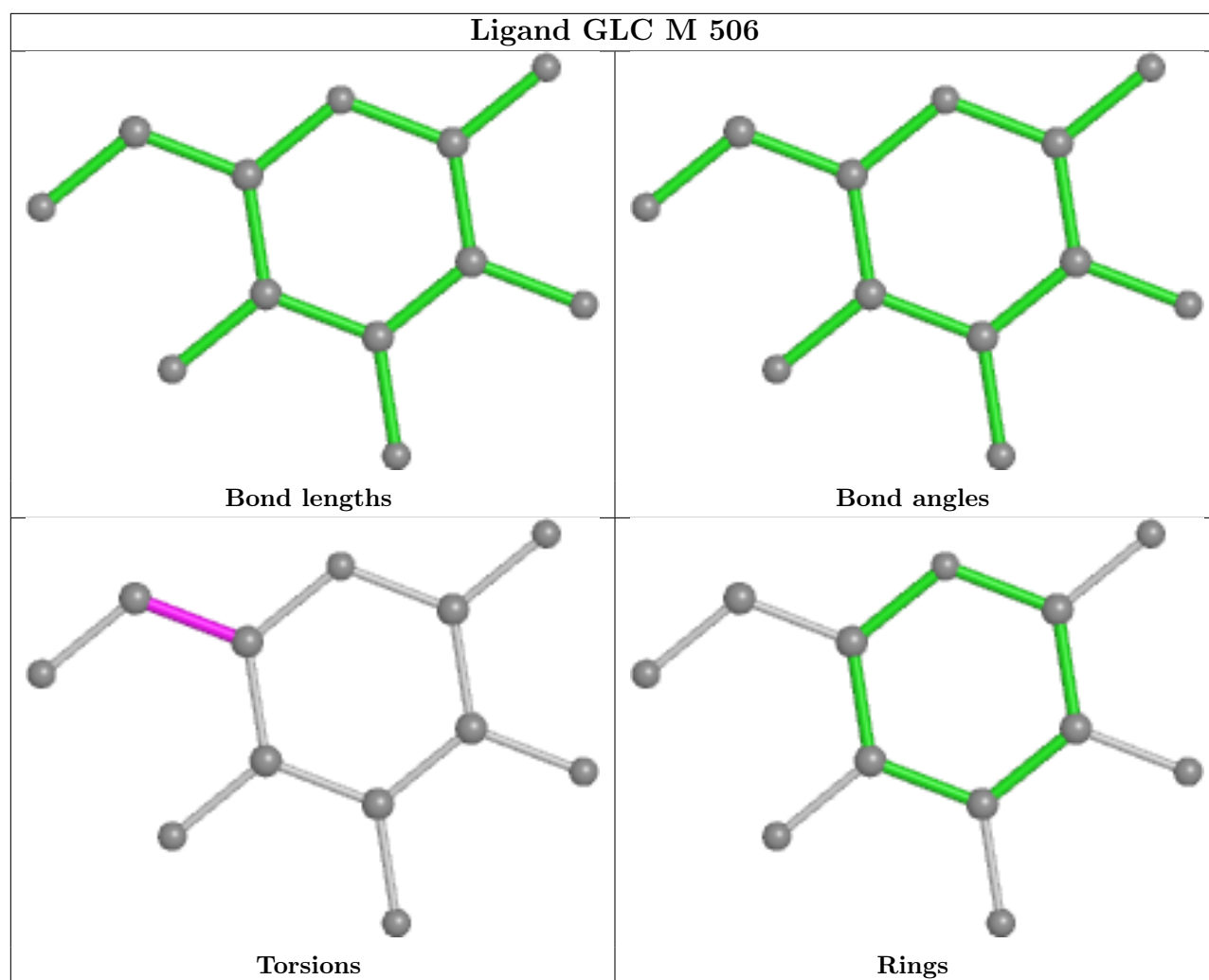
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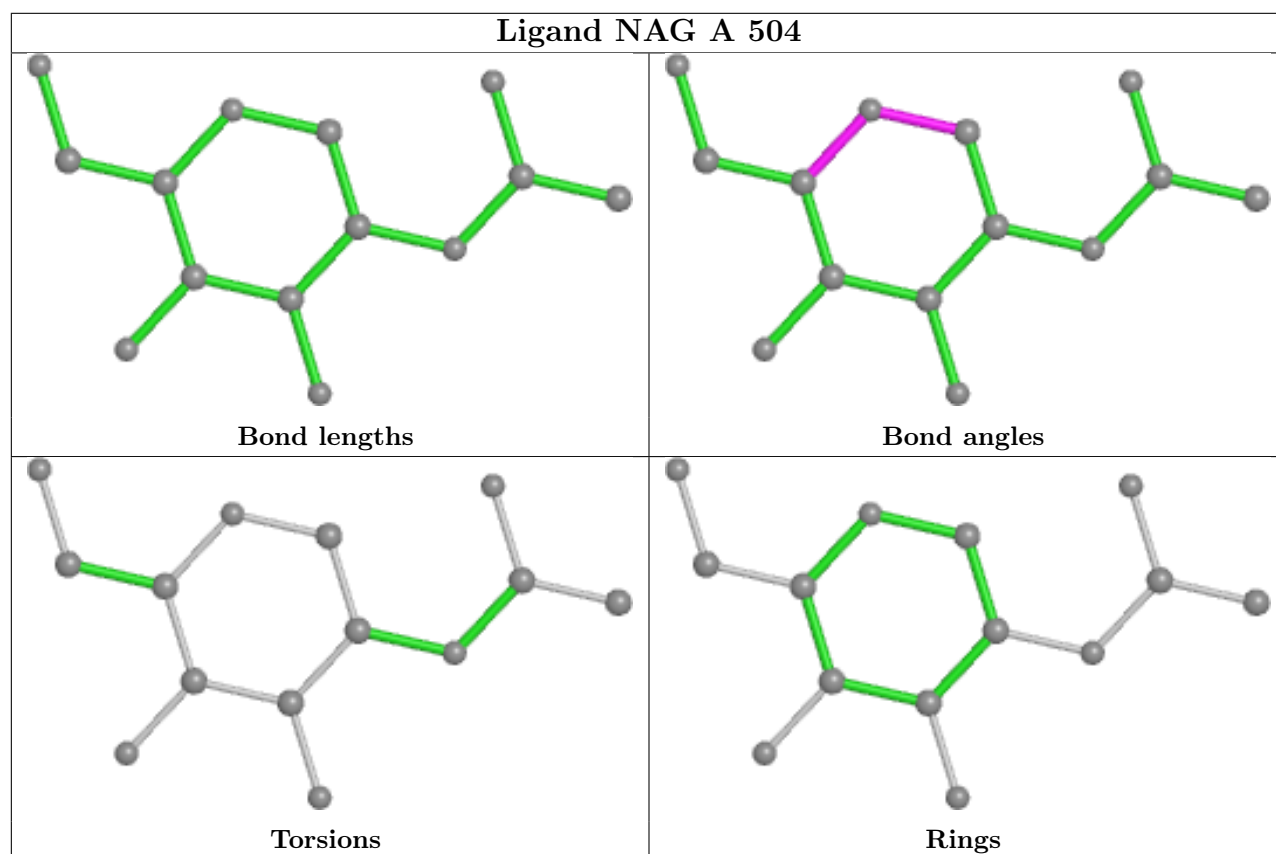
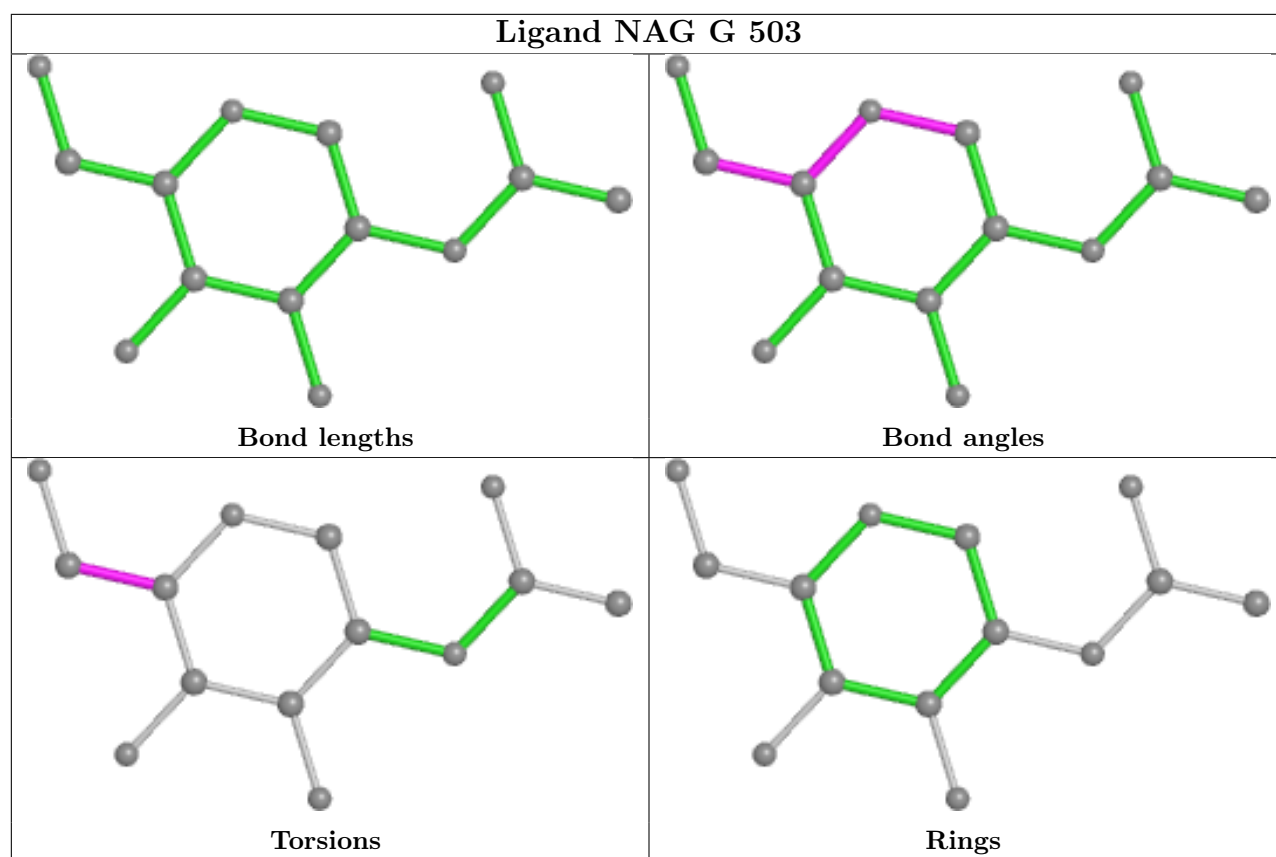


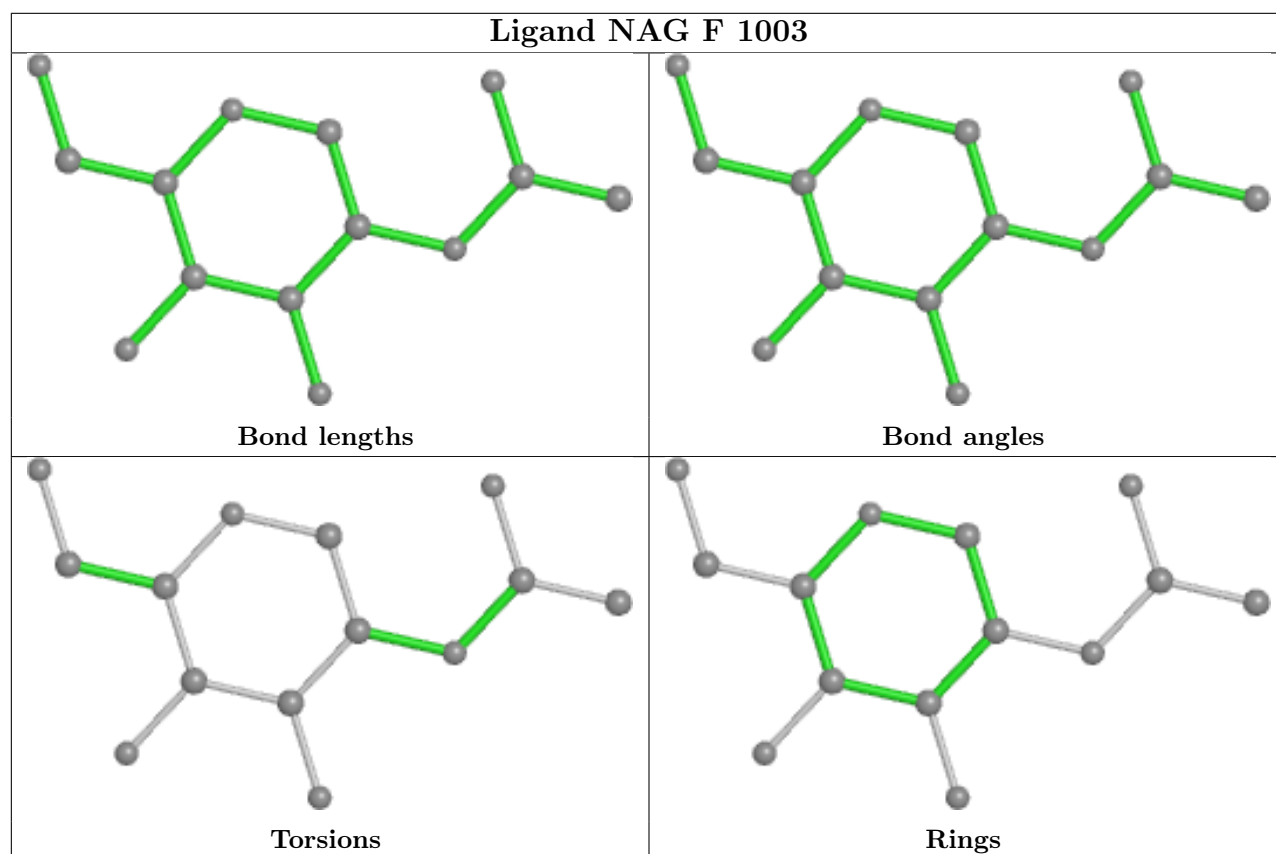
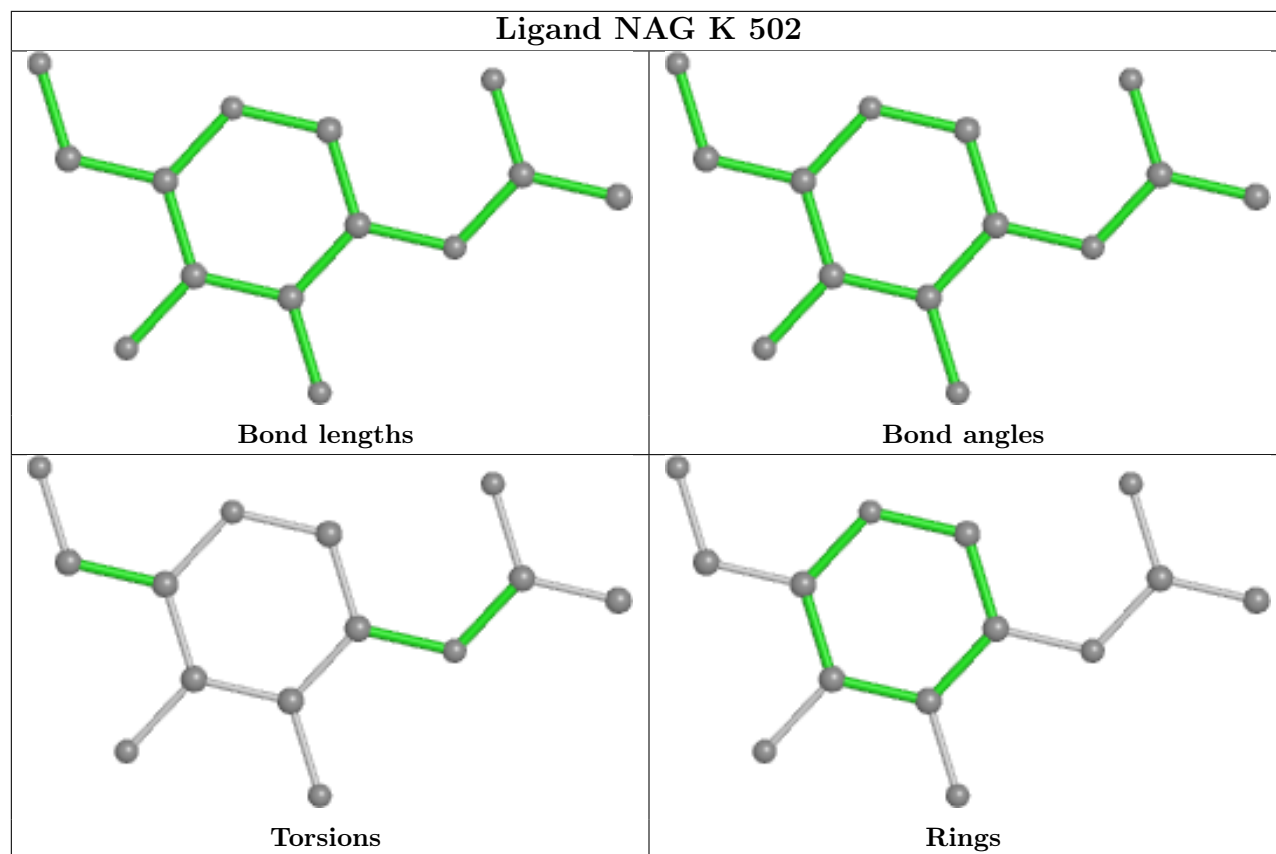
Ligand NAG I 502

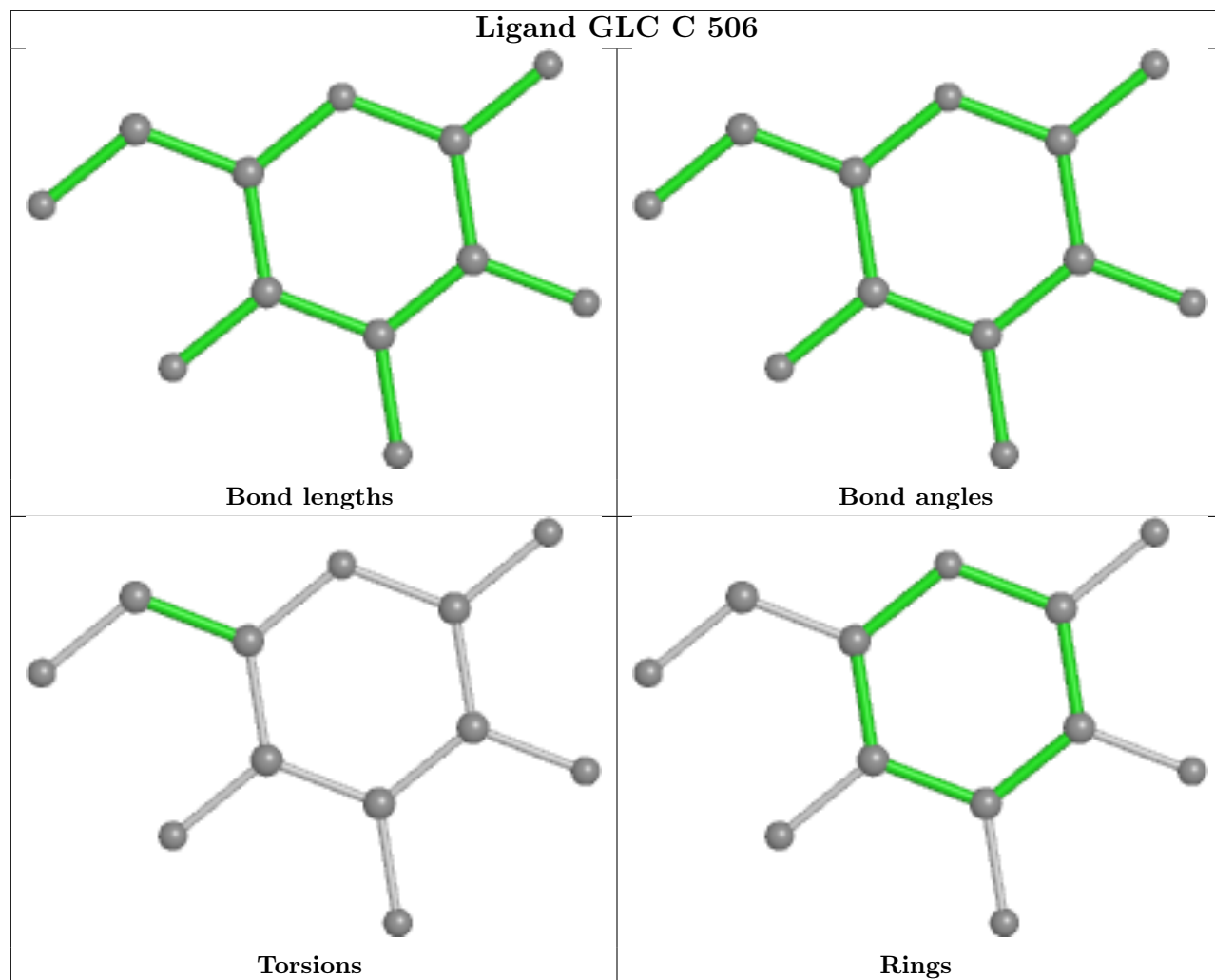


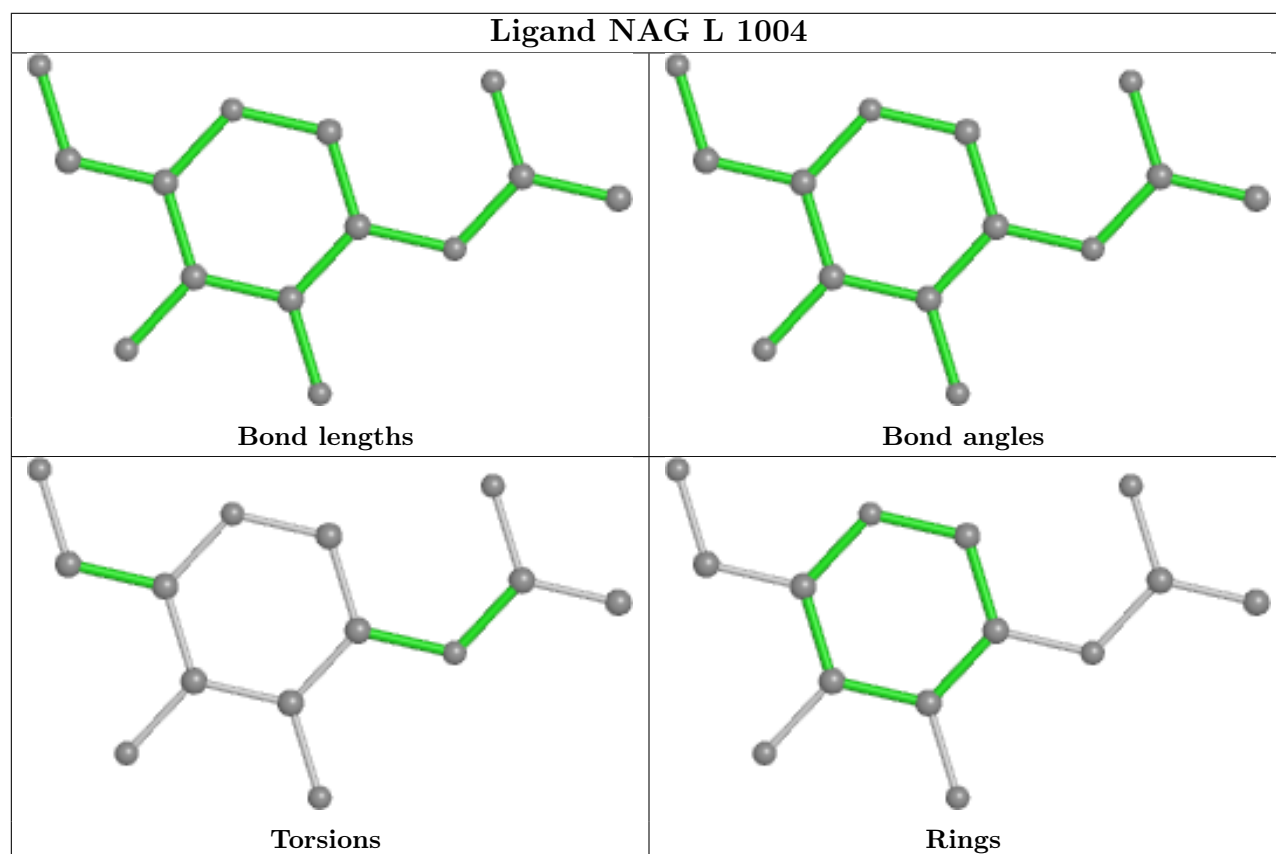
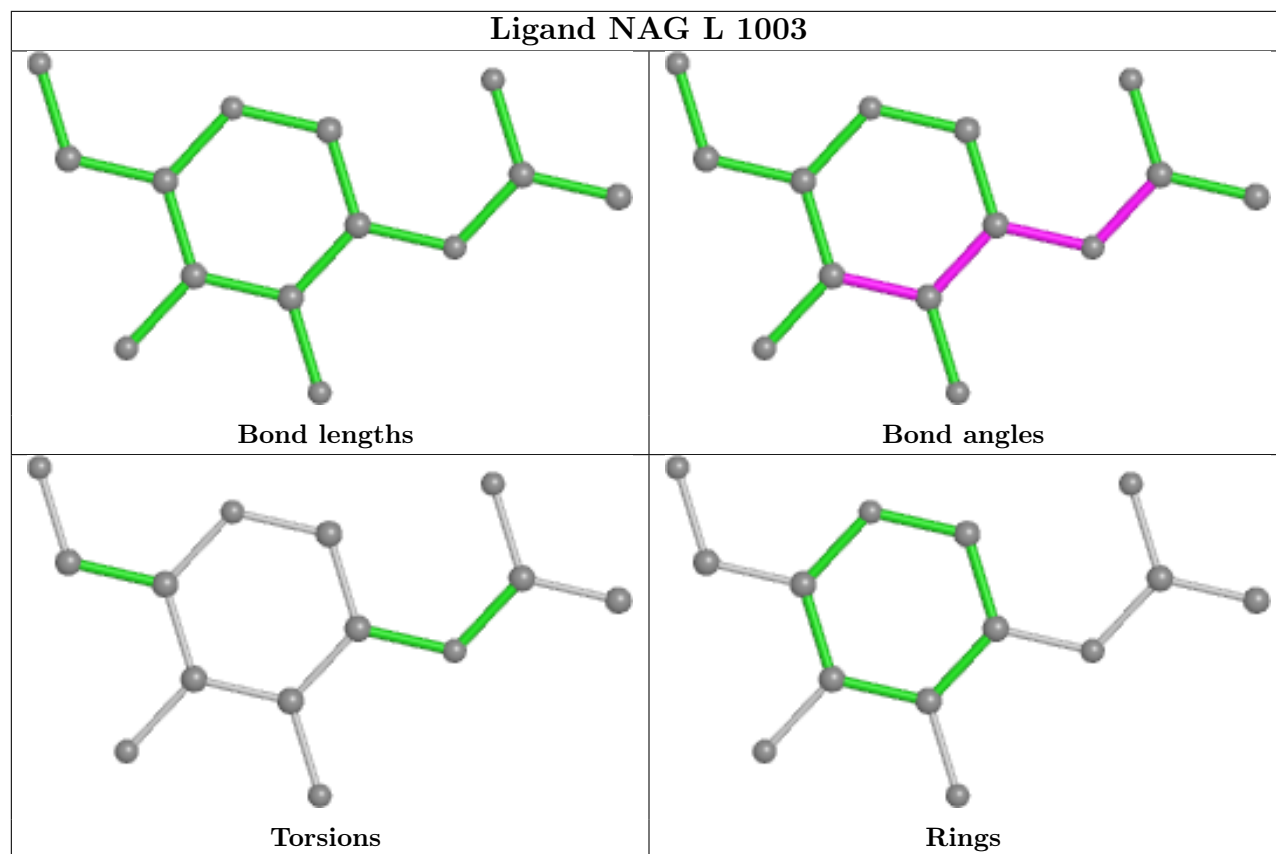


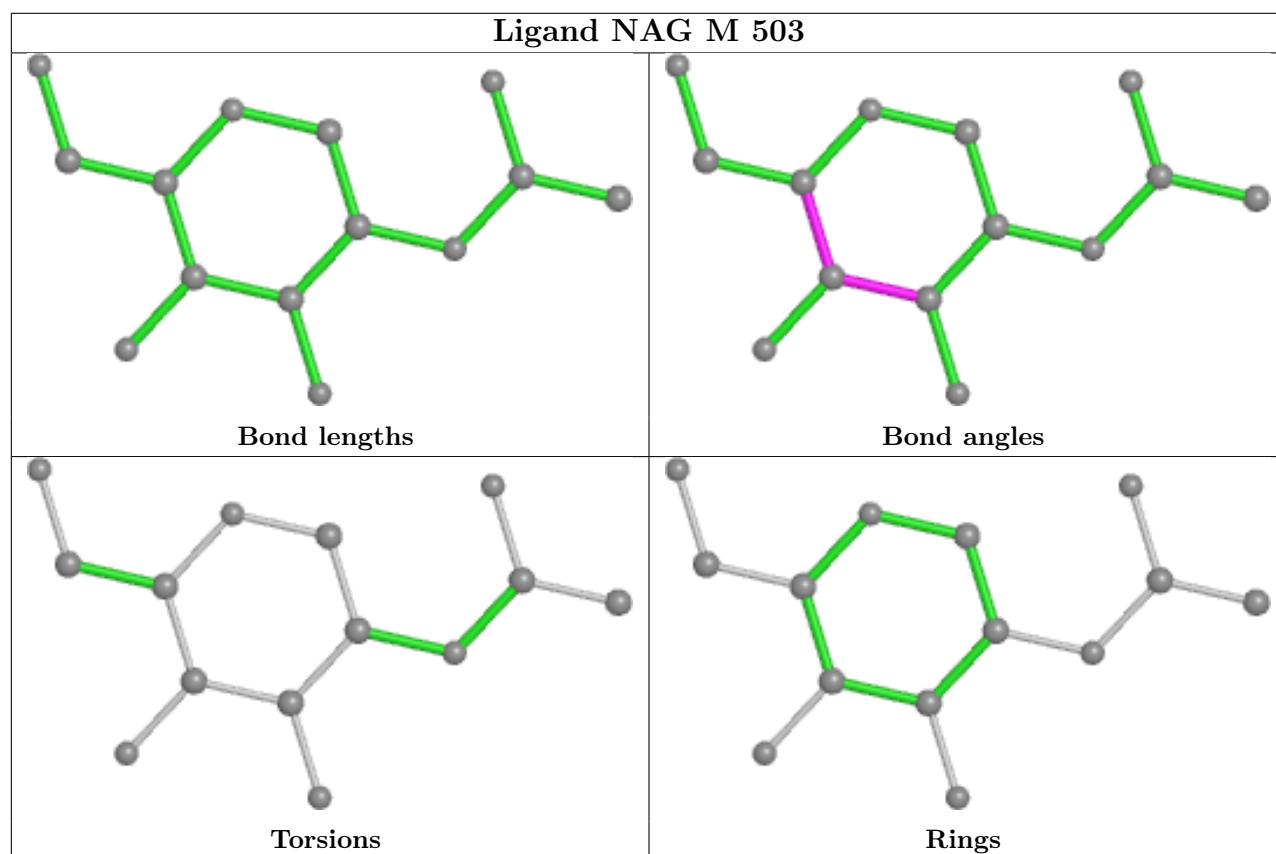
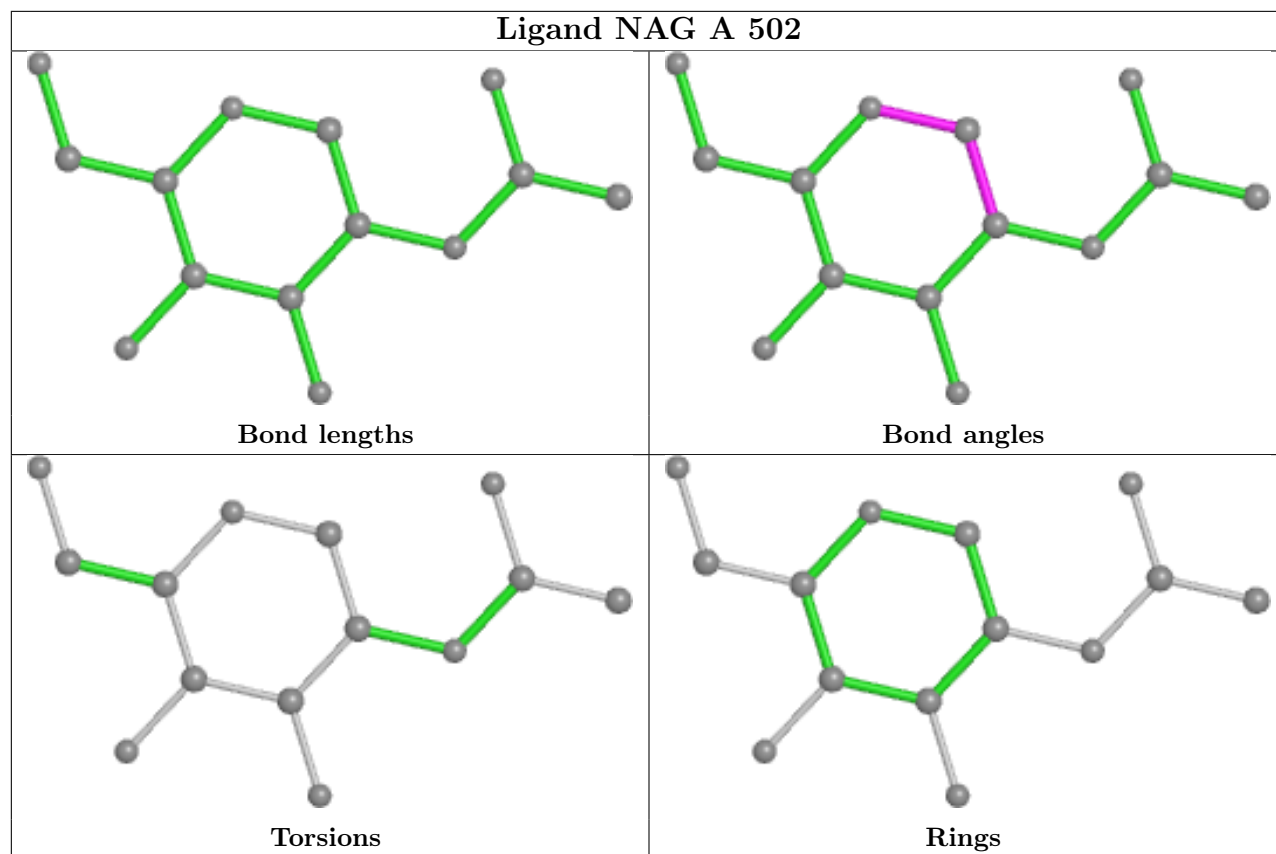












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	465/548 (84%)	-0.36	0 100 100	22, 32, 42, 72	0
1	C	465/548 (84%)	-0.28	1 (0%) 95 96	25, 36, 49, 65	0
1	E	465/548 (84%)	-0.32	2 (0%) 92 95	24, 34, 46, 70	0
1	G	465/548 (84%)	-0.33	3 (0%) 89 92	24, 34, 46, 66	0
1	I	465/548 (84%)	-0.36	0 100 100	23, 33, 46, 65	0
1	K	465/548 (84%)	-0.37	0 100 100	24, 34, 45, 64	0
1	M	465/548 (84%)	-0.37	0 100 100	22, 32, 42, 68	0
1	O	465/548 (84%)	-0.30	1 (0%) 95 96	25, 36, 49, 70	0
2	B	436/445 (97%)	-0.32	3 (0%) 87 91	22, 31, 51, 83	0
2	D	436/445 (97%)	-0.25	3 (0%) 87 91	25, 34, 55, 91	0
2	F	436/445 (97%)	-0.27	7 (1%) 72 77	24, 32, 52, 85	0
2	H	436/445 (97%)	-0.28	5 (1%) 80 85	25, 34, 56, 85	0
2	J	436/445 (97%)	-0.20	6 (1%) 75 80	22, 34, 58, 91	0
2	L	436/445 (97%)	-0.17	4 (0%) 84 88	25, 35, 59, 83	0
2	N	436/445 (97%)	-0.24	4 (0%) 84 88	22, 33, 53, 83	0
2	P	436/445 (97%)	-0.17	3 (0%) 87 91	26, 37, 61, 90	0
All	All	7208/7944 (90%)	-0.29	42 (0%) 89 92	22, 34, 51, 91	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	516	SER	4.9
1	G	31	PRO	4.0
2	H	517	ARG	3.6
2	D	705	TYR	3.5
2	D	534	PRO	3.4

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	b	3	11/12	0.78	0.18	62,64,65,66	0
5	BMA	r	3	11/12	0.78	0.17	60,63,64,65	0
5	BMA	T	3	11/12	0.81	0.17	59,60,62,64	0
5	BMA	f	3	11/12	0.84	0.16	56,61,65,65	0
5	BMA	X	3	11/12	0.84	0.16	55,58,60,64	0
4	NAG	V	2	14/15	0.85	0.19	50,56,61,62	0
5	BMA	v	3	11/12	0.85	0.16	62,65,68,70	0
5	BMA	n	3	11/12	0.86	0.15	61,63,65,68	0
5	BMA	j	3	11/12	0.88	0.18	63,66,67,68	0
4	NAG	Z	2	14/15	0.89	0.22	51,56,60,60	0
4	NAG	p	2	14/15	0.90	0.19	52,55,58,59	0
4	NAG	R	2	14/15	0.91	0.11	45,48,49,52	0
4	NAG	l	2	14/15	0.91	0.14	48,50,54,55	0
3	GLC	m	1	12/12	0.91	0.14	38,43,44,44	0
4	NAG	t	2	14/15	0.91	0.17	51,59,62,64	0
4	NAG	d	2	14/15	0.92	0.15	51,53,55,56	0
4	NAG	h	2	14/15	0.92	0.13	46,50,51,54	0
5	NAG	X	2	14/15	0.92	0.14	37,45,49,53	0
5	NAG	r	2	14/15	0.92	0.16	42,47,52,58	0
3	GLC	U	2	11/12	0.92	0.11	39,43,47,48	0
3	GLC	W	2	11/12	0.92	0.11	43,45,46,47	0
5	NAG	n	2	14/15	0.93	0.14	45,50,53,56	0
3	GLC	s	2	11/12	0.93	0.14	41,43,45,45	0
5	NAG	T	2	14/15	0.93	0.13	38,45,49,55	0
4	NAG	V	1	14/15	0.93	0.12	36,42,45,49	0
4	NAG	t	1	14/15	0.93	0.15	42,49,54,54	0
3	GLC	c	2	11/12	0.94	0.11	37,39,40,40	0
5	NAG	f	2	14/15	0.94	0.12	42,45,49,54	0
3	GLC	u	2	11/12	0.94	0.14	48,49,50,51	0
3	GLC	g	2	11/12	0.94	0.12	33,34,35,36	0
3	GLC	k	2	11/12	0.94	0.12	37,39,40,40	0
3	GLC	a	2	11/12	0.94	0.13	42,43,44,44	0

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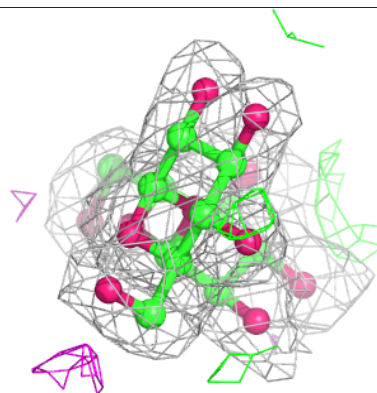
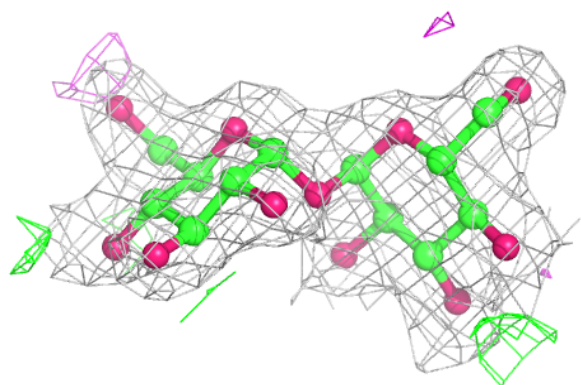
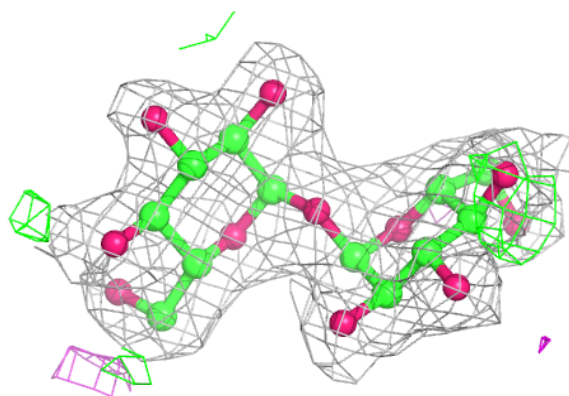
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLC	m	2	11/12	0.94	0.10	41,43,44,44	0
3	GLC	o	2	11/12	0.94	0.11	37,37,38,39	0
3	GLC	q	1	12/12	0.94	0.13	37,40,42,43	0
3	GLC	u	1	12/12	0.95	0.15	43,46,47,49	0
4	NAG	h	1	14/15	0.95	0.12	37,40,42,44	0
5	NAG	b	2	14/15	0.95	0.11	38,44,49,56	0
3	GLC	i	2	11/12	0.95	0.13	43,44,45,46	0
4	NAG	l	1	14/15	0.95	0.12	36,38,40,42	0
3	GLC	k	1	12/12	0.95	0.13	33,35,37,37	0
5	NAG	j	2	14/15	0.95	0.13	46,49,54,59	0
4	NAG	p	1	14/15	0.95	0.12	41,43,45,48	0
3	GLC	Q	2	11/12	0.95	0.10	33,34,36,37	0
3	GLC	q	2	11/12	0.95	0.14	39,41,41,42	0
4	NAG	Z	1	14/15	0.95	0.12	39,40,44,47	0
3	GLC	i	1	12/12	0.95	0.14	40,42,43,44	0
4	NAG	d	1	14/15	0.95	0.16	39,40,46,47	0
4	NAG	R	1	14/15	0.96	0.11	35,36,39,41	0
5	NAG	f	1	14/15	0.96	0.10	31,34,35,39	0
3	GLC	a	1	12/12	0.96	0.14	36,37,38,39	0
5	NAG	T	1	14/15	0.96	0.12	28,31,33,38	0
3	GLC	W	1	12/12	0.96	0.12	35,38,38,39	0
3	GLC	c	1	12/12	0.96	0.12	37,38,39,40	0
5	NAG	n	1	14/15	0.96	0.12	35,38,43,44	0
5	NAG	X	1	14/15	0.96	0.11	33,36,39,39	0
3	GLC	U	1	12/12	0.96	0.09	39,40,42,43	0
5	NAG	r	1	14/15	0.96	0.10	32,36,38,41	0
3	GLC	e	1	12/12	0.96	0.11	38,40,40,41	0
5	NAG	b	1	14/15	0.96	0.12	28,30,33,36	0
5	NAG	v	2	14/15	0.96	0.15	41,48,53,59	0
3	GLC	Y	2	11/12	0.96	0.09	34,37,38,38	0
3	GLC	g	1	12/12	0.97	0.09	30,33,34,36	0
3	GLC	Q	1	12/12	0.97	0.10	32,35,36,38	0
3	GLC	o	1	12/12	0.97	0.09	28,31,32,34	0
3	GLC	Y	1	12/12	0.97	0.11	32,36,36,37	0
3	GLC	S	1	12/12	0.97	0.10	32,33,35,36	0
3	GLC	S	2	11/12	0.97	0.10	36,38,39,40	0
5	NAG	v	1	14/15	0.97	0.09	31,37,39,42	0
3	GLC	s	1	12/12	0.97	0.10	32,36,37,38	0
3	GLC	e	2	11/12	0.97	0.09	41,43,44,44	0
5	NAG	j	1	14/15	0.98	0.10	31,36,38,41	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

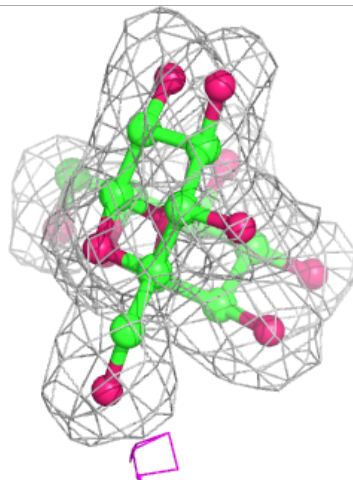
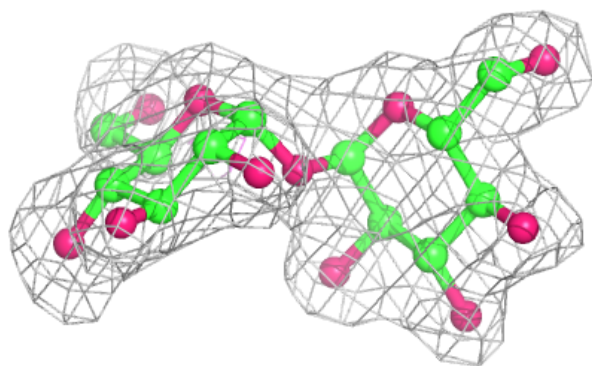
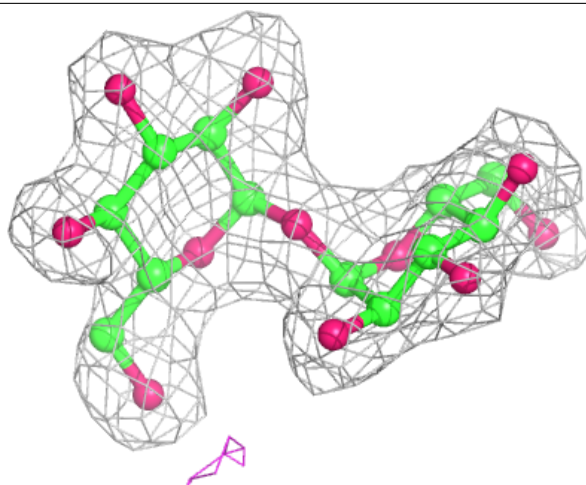
Electron density around Chain Q:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



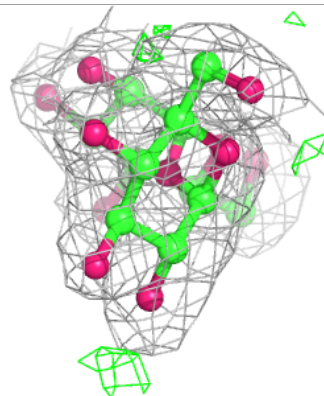
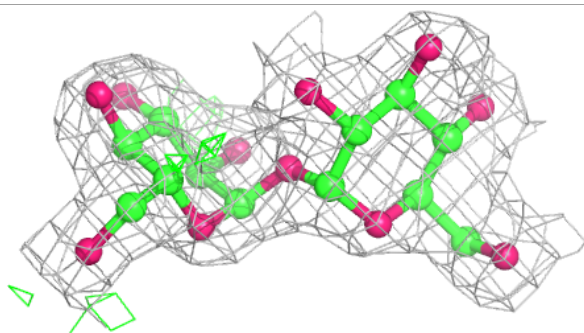
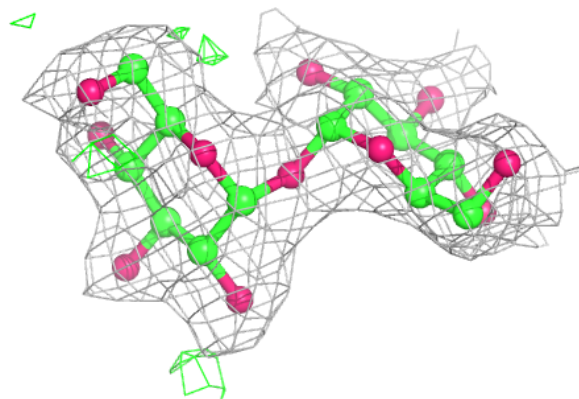
Electron density around Chain S:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

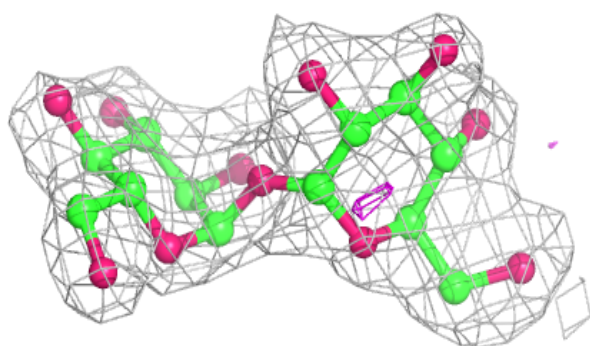
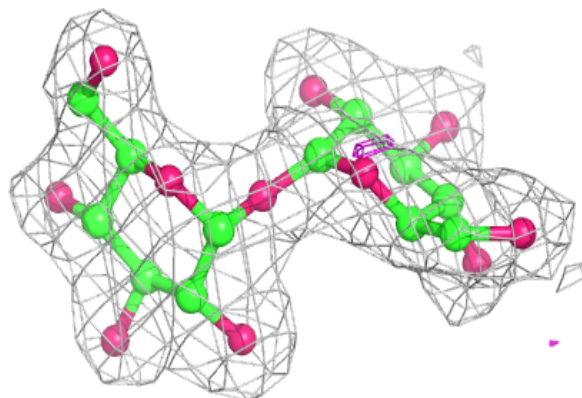


Electron density around Chain U:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

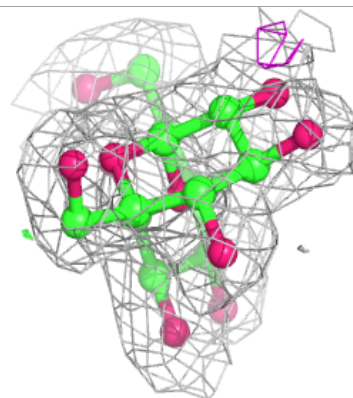
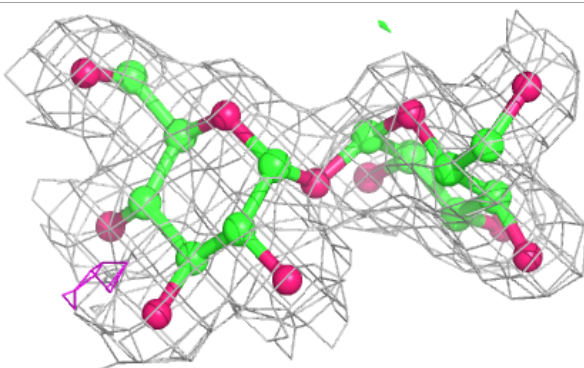
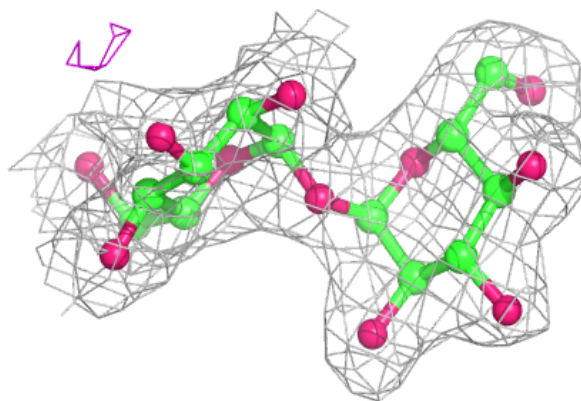
**Electron density around Chain W:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

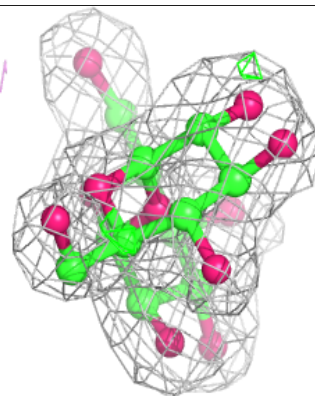
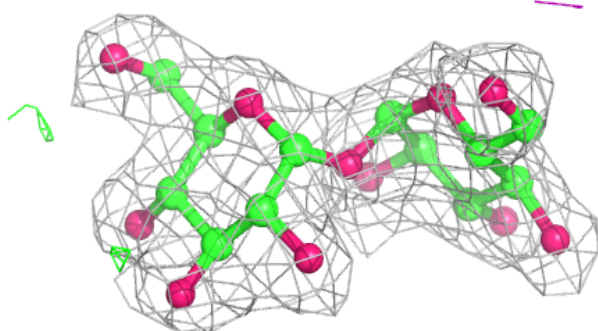
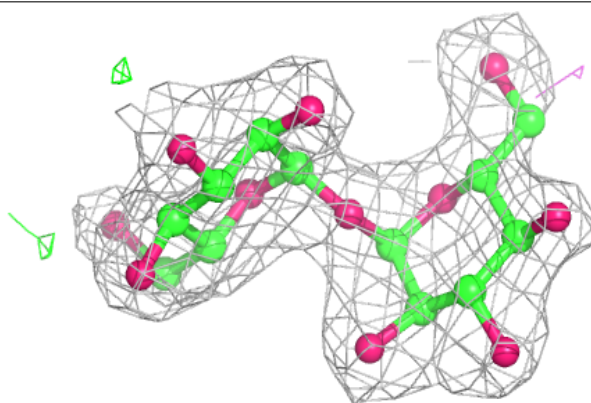


Electron density around Chain Y:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

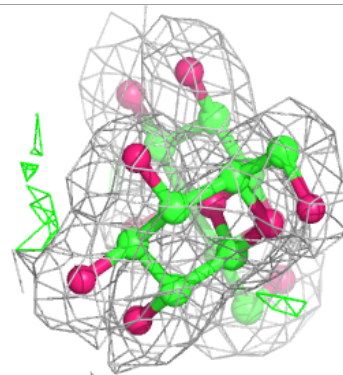
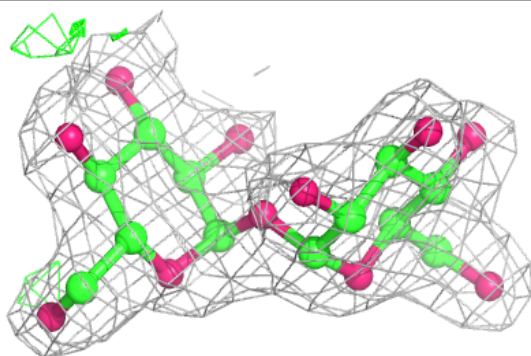
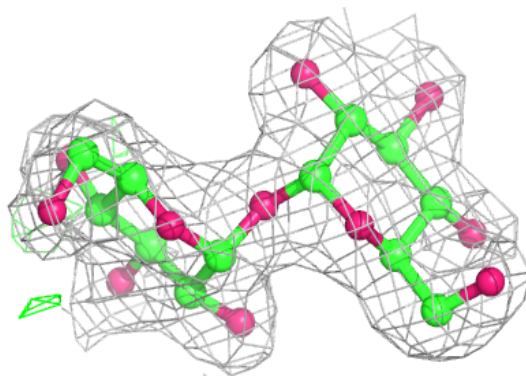
**Electron density around Chain a:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



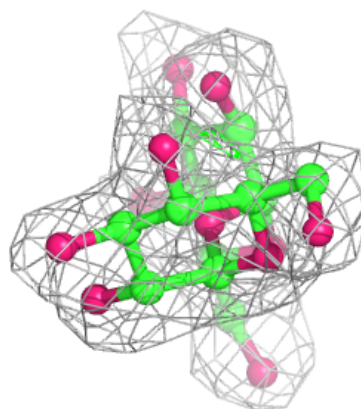
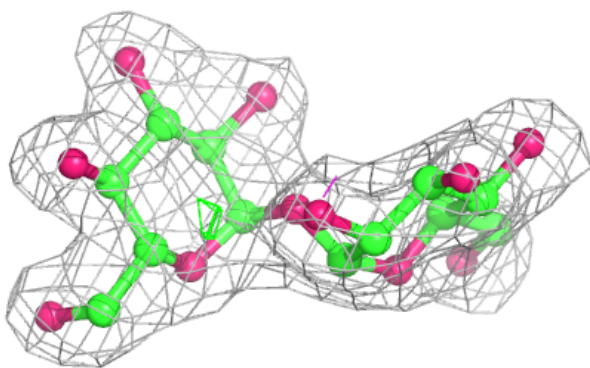
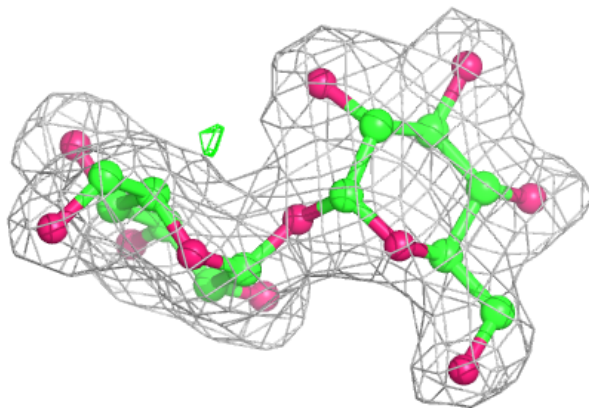
Electron density around Chain c:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



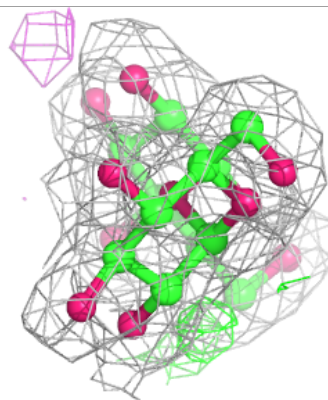
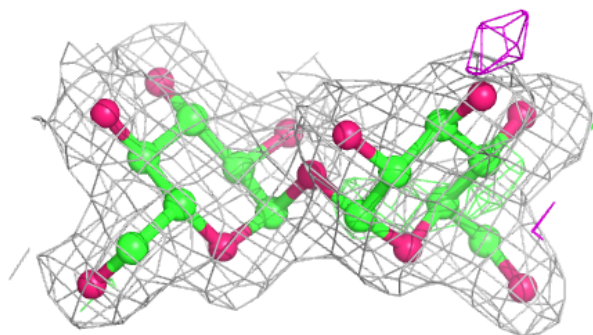
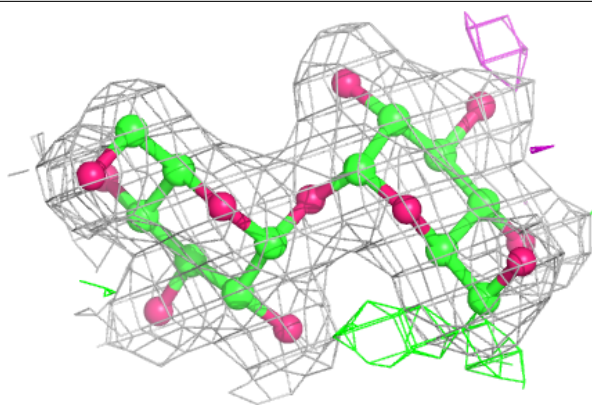
Electron density around Chain e:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



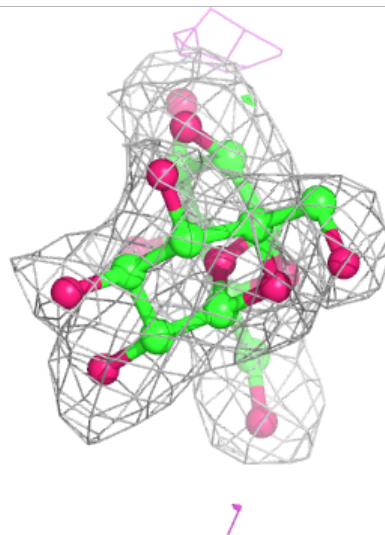
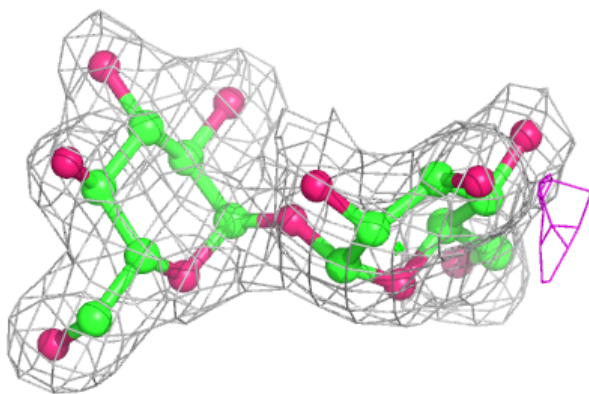
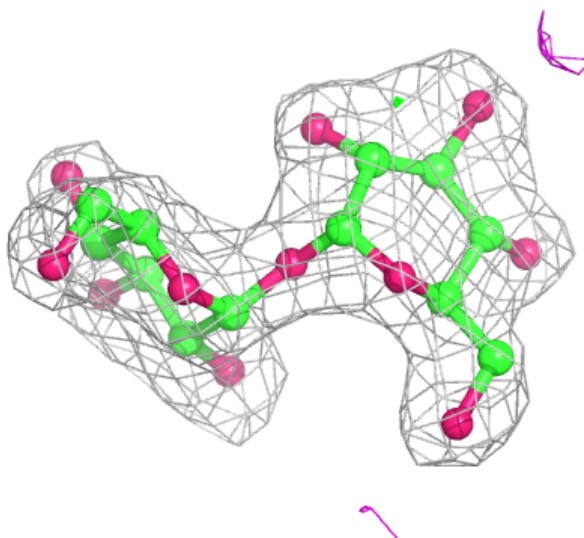
Electron density around Chain g:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



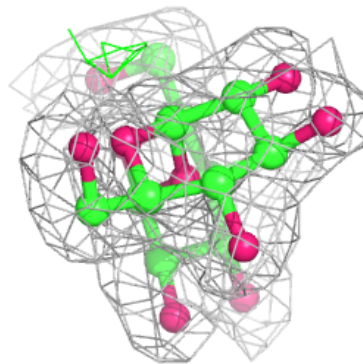
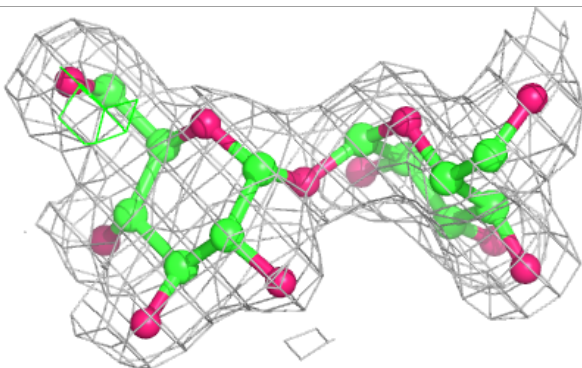
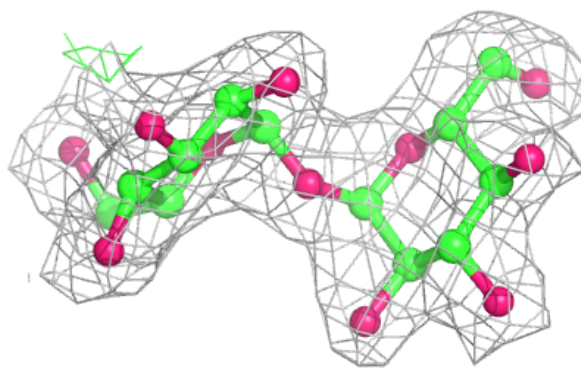
Electron density around Chain i:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

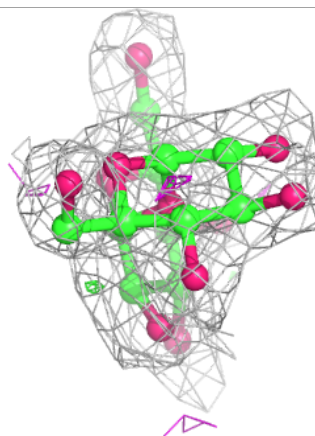
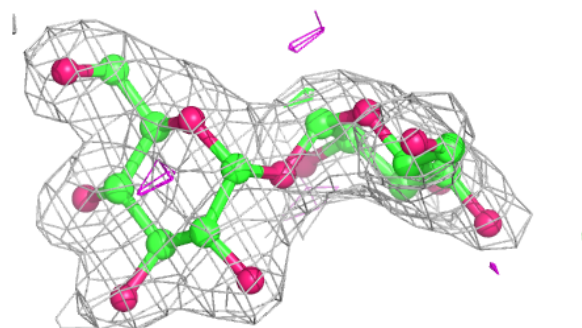
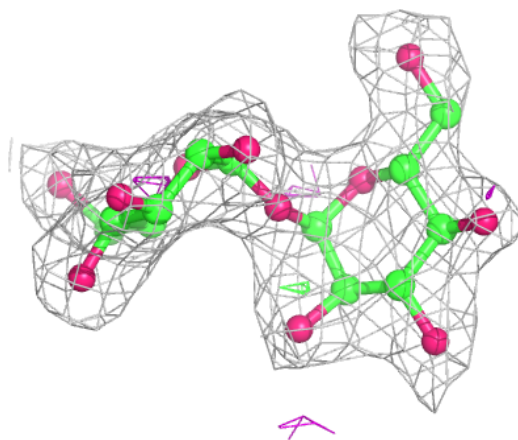


Electron density around Chain k:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

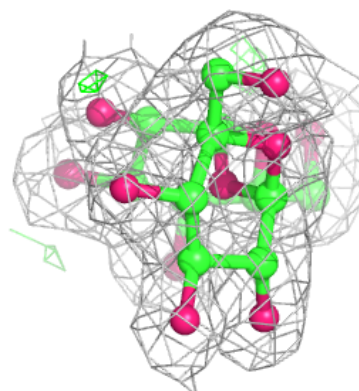
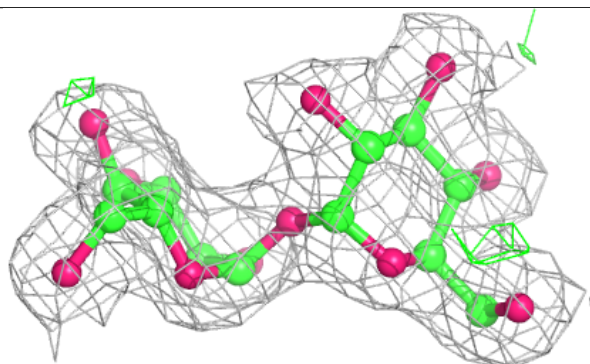
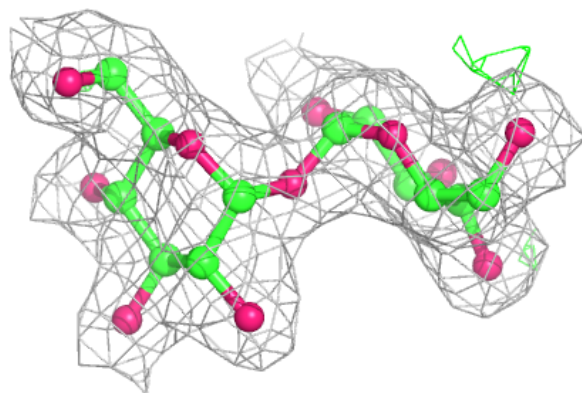
**Electron density around Chain m:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

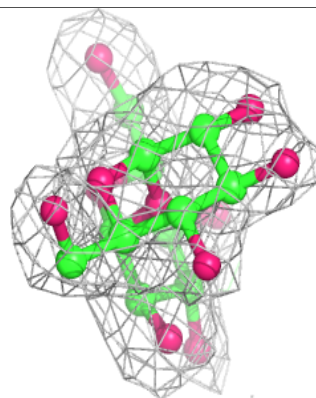
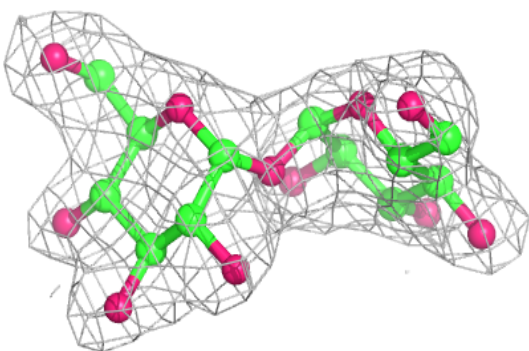
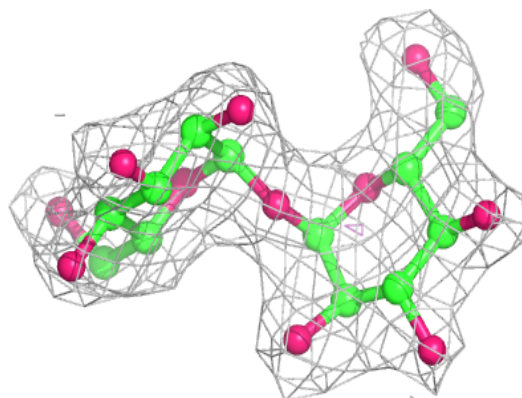


Electron density around Chain o:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

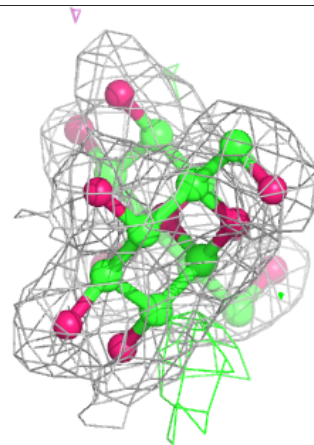
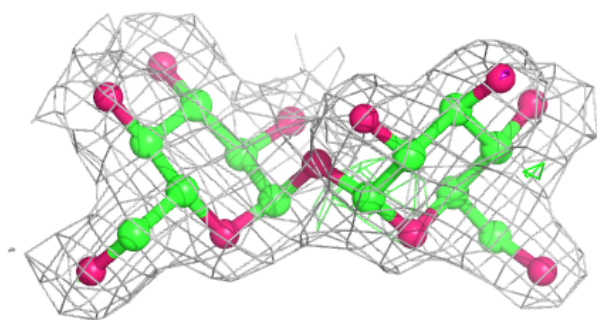
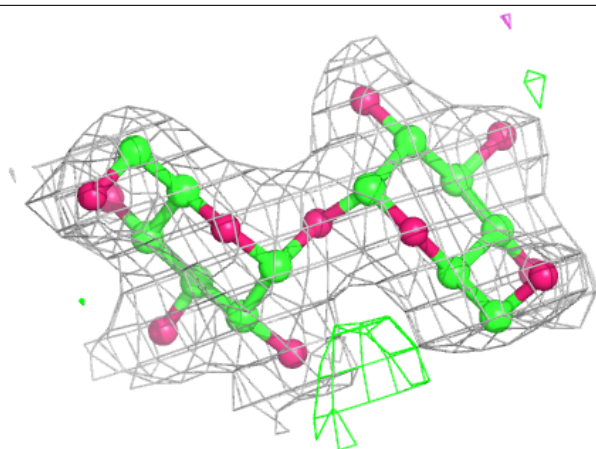
**Electron density around Chain q:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



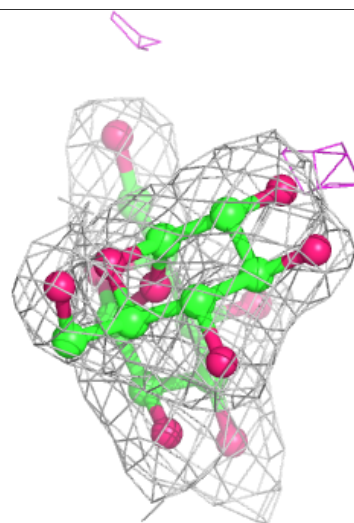
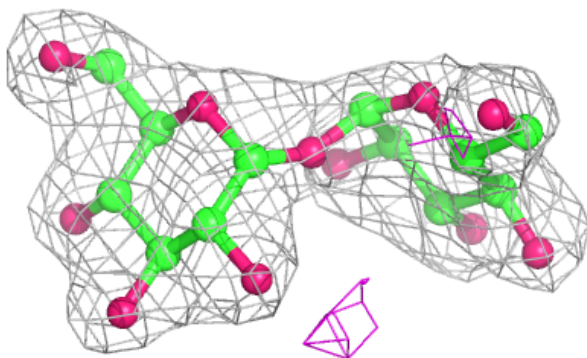
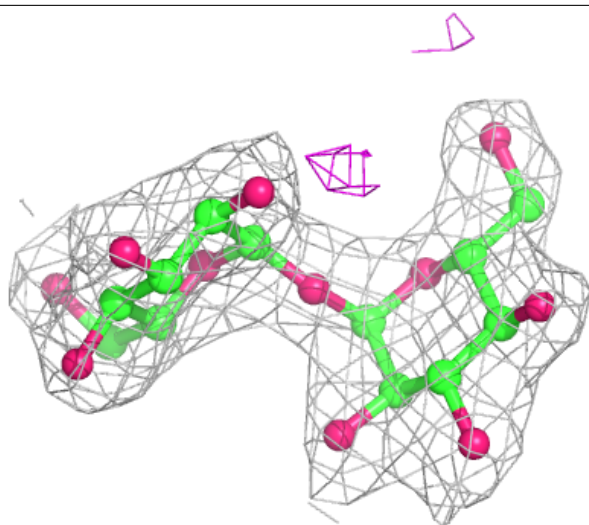
Electron density around Chain s:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



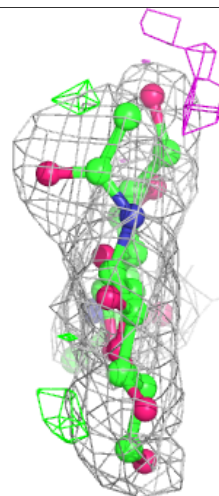
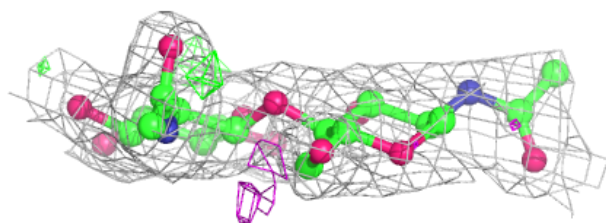
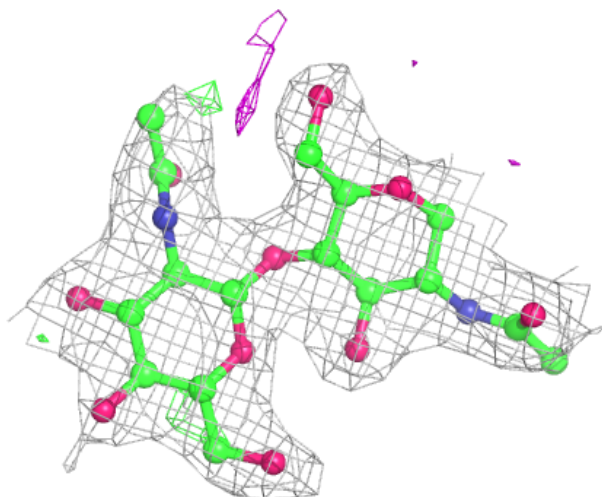
Electron density around Chain u:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



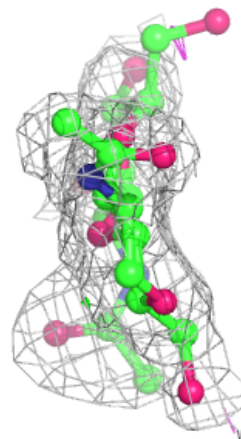
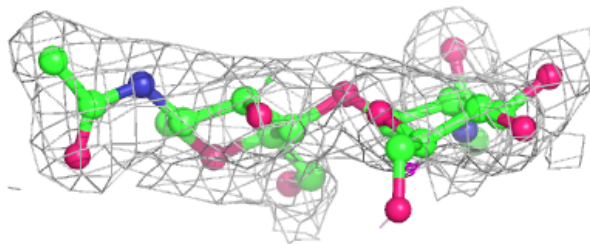
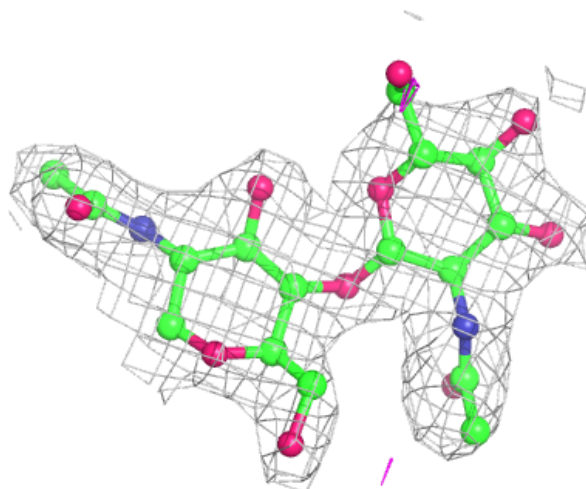
Electron density around Chain R:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



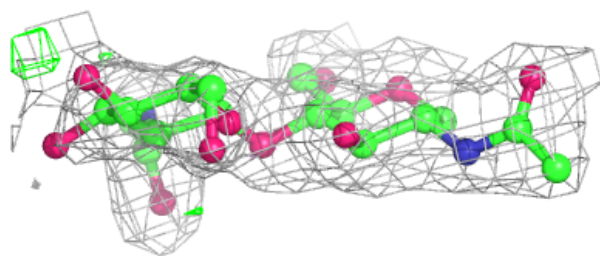
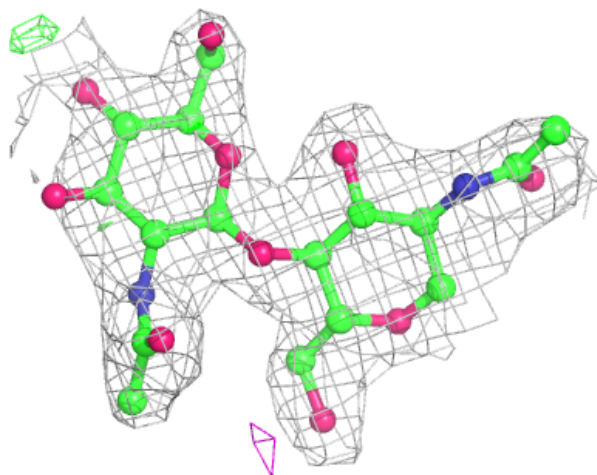
Electron density around Chain V:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



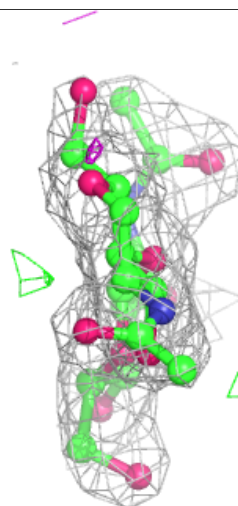
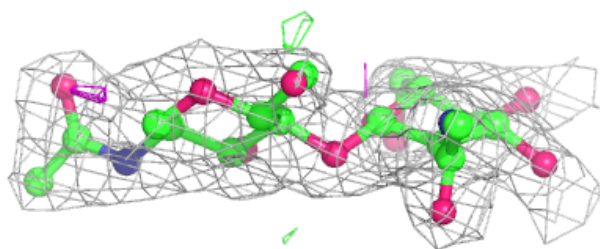
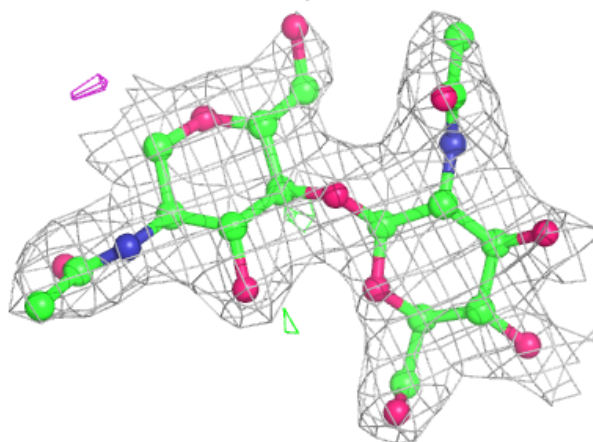
Electron density around Chain Z:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



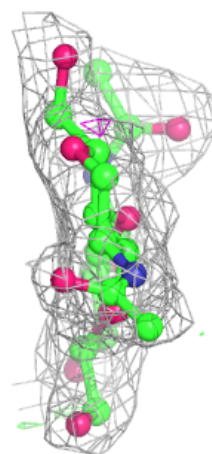
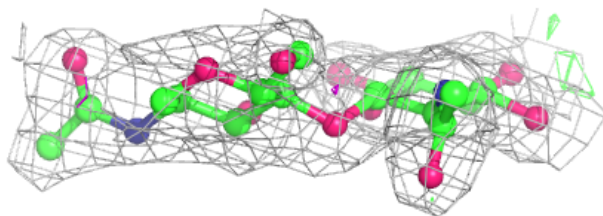
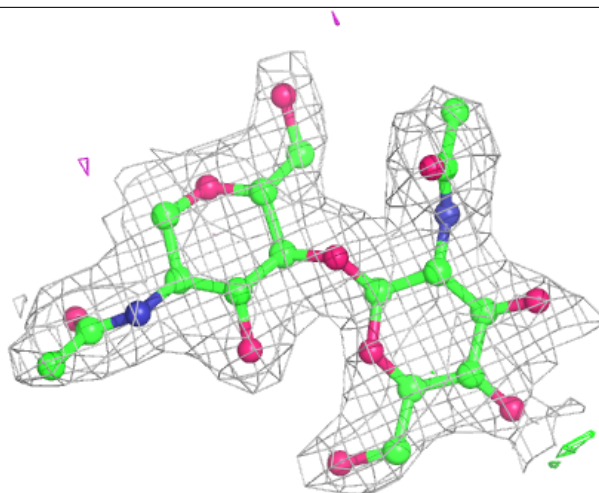
Electron density around Chain d:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



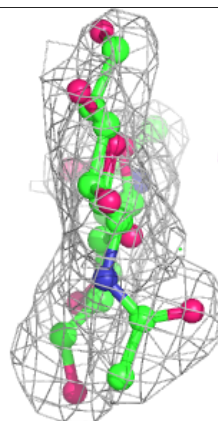
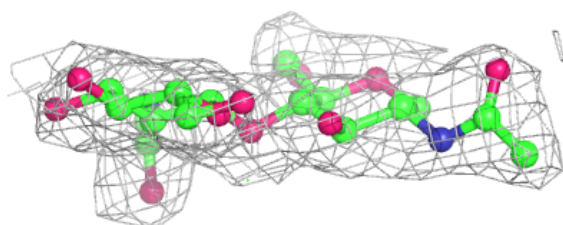
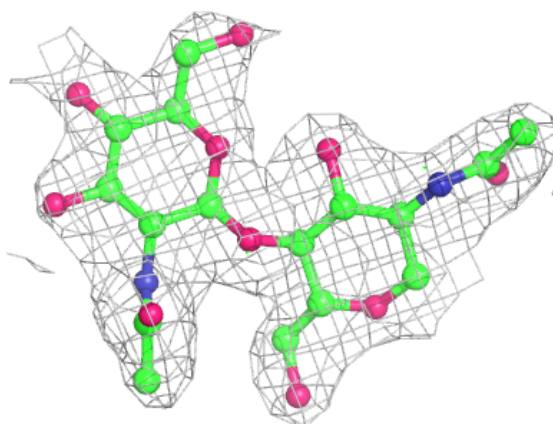
Electron density around Chain h:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



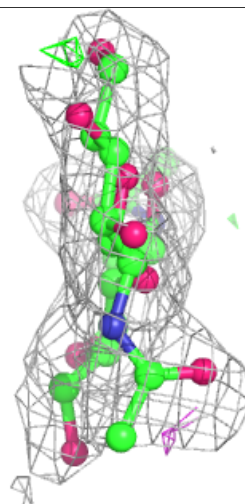
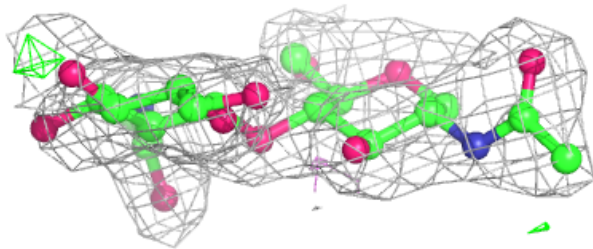
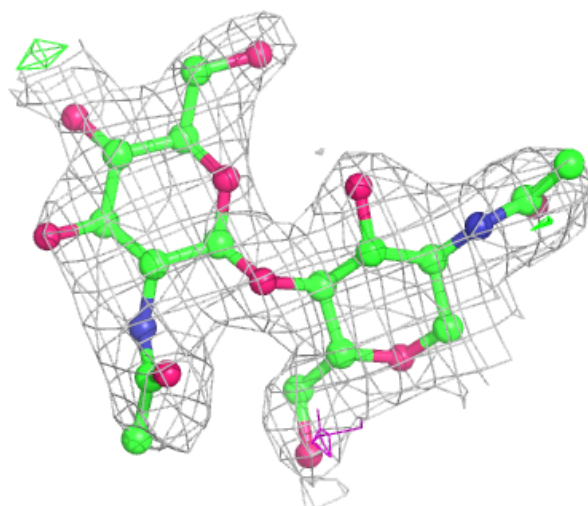
Electron density around Chain 1:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



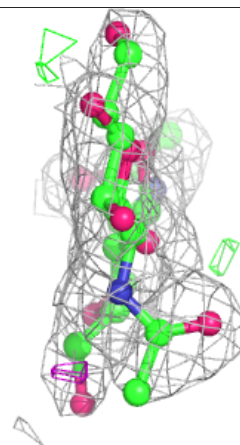
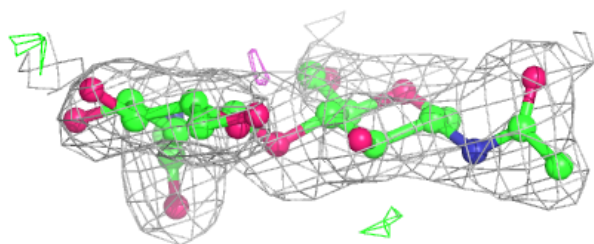
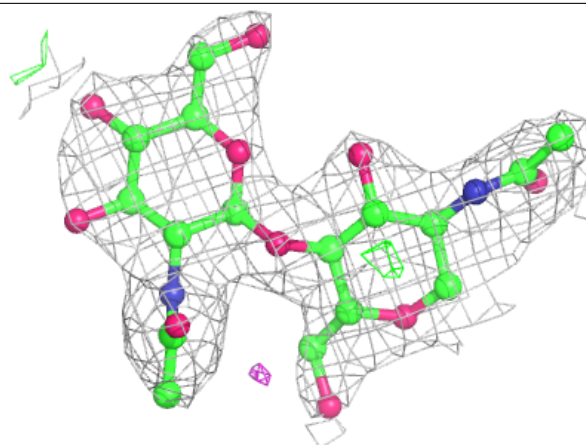
Electron density around Chain p:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



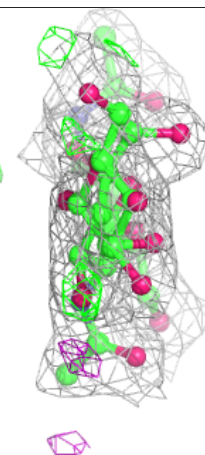
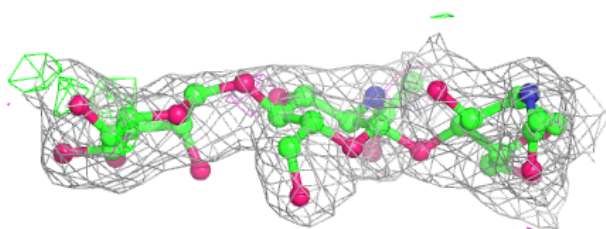
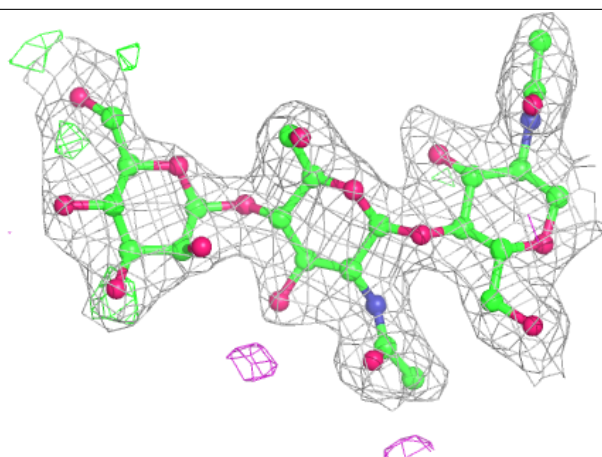
Electron density around Chain t:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



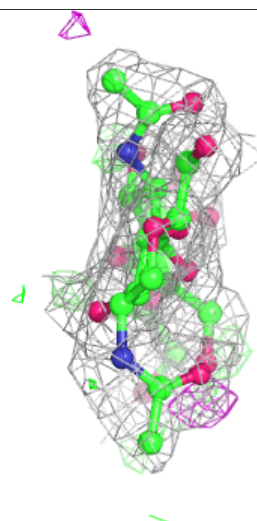
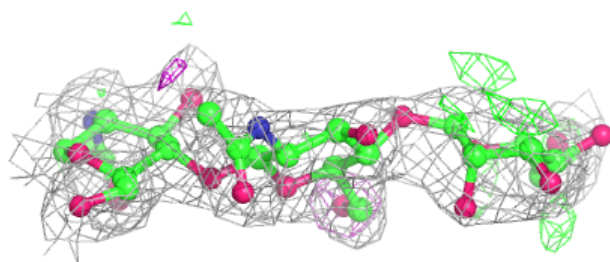
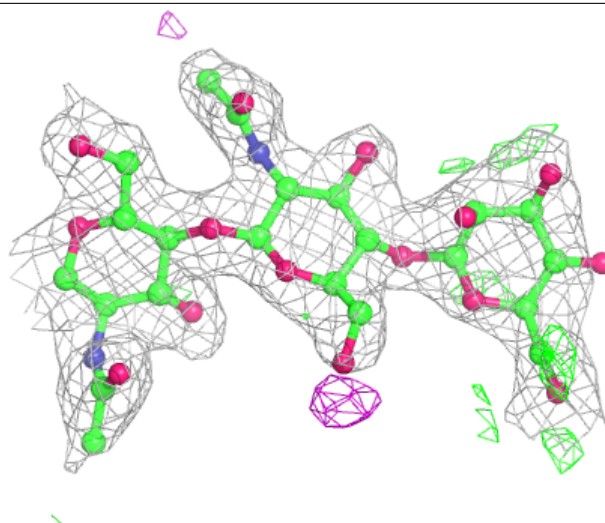
Electron density around Chain T:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



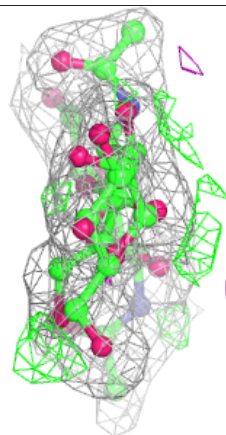
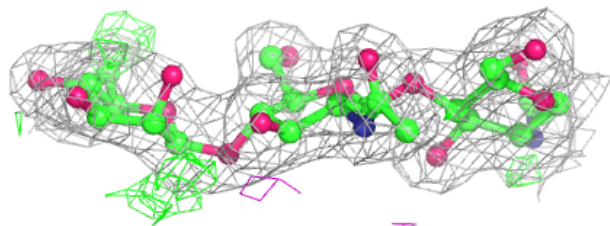
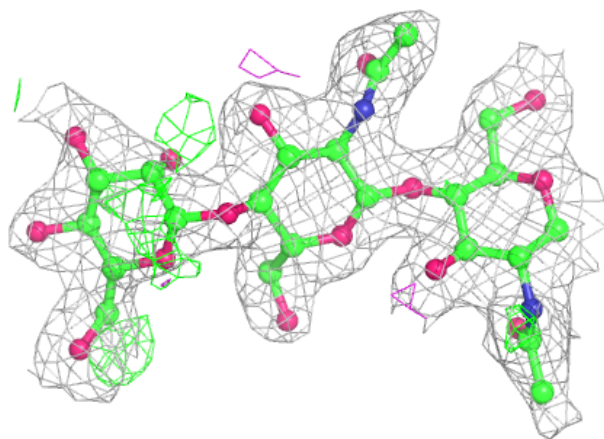
Electron density around Chain X:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



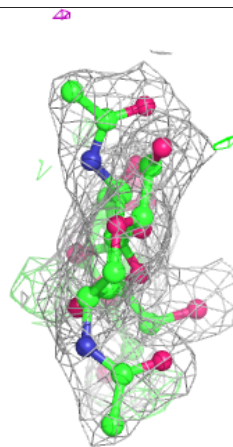
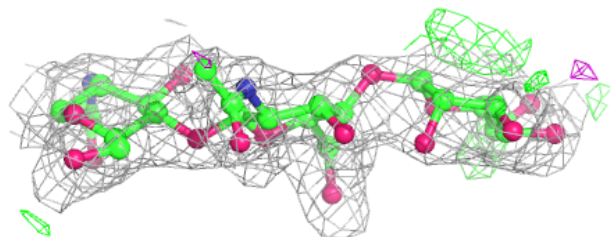
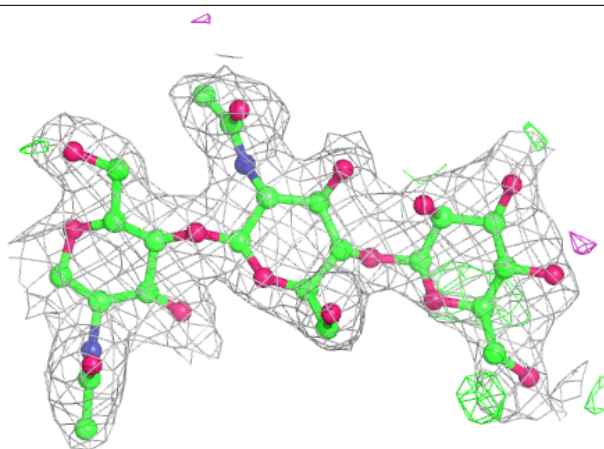
Electron density around Chain b:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



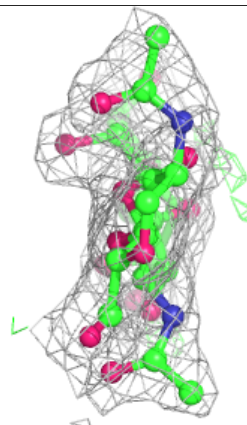
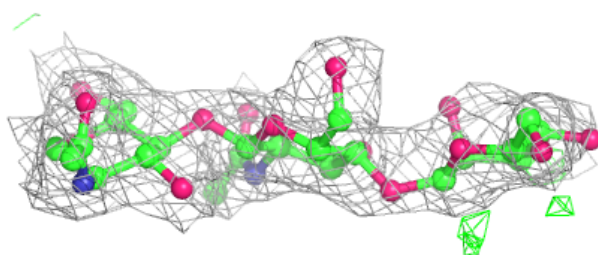
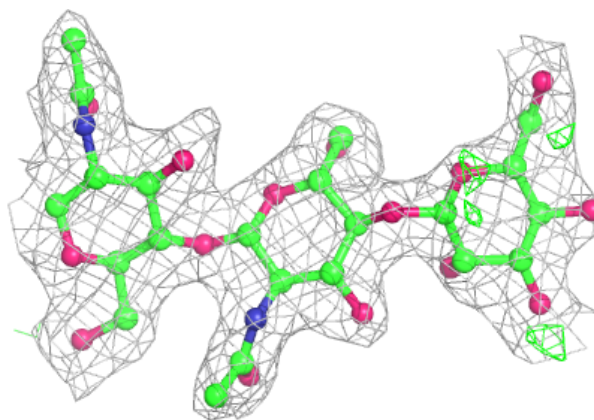
Electron density around Chain f:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



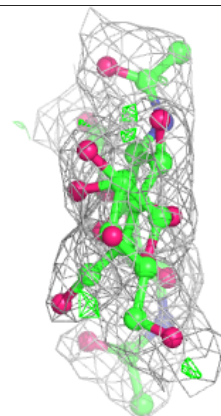
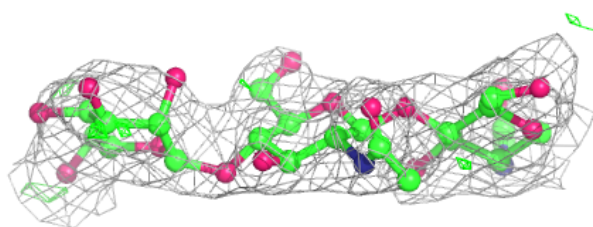
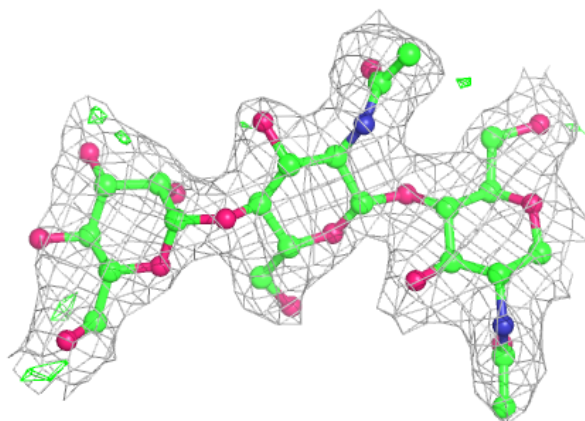
Electron density around Chain j:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

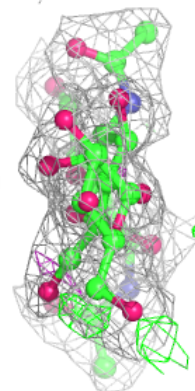
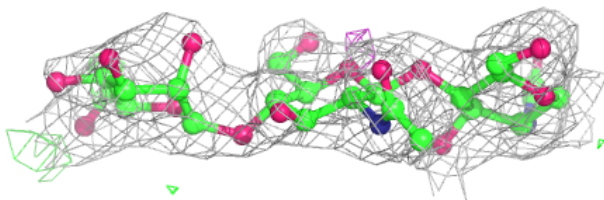
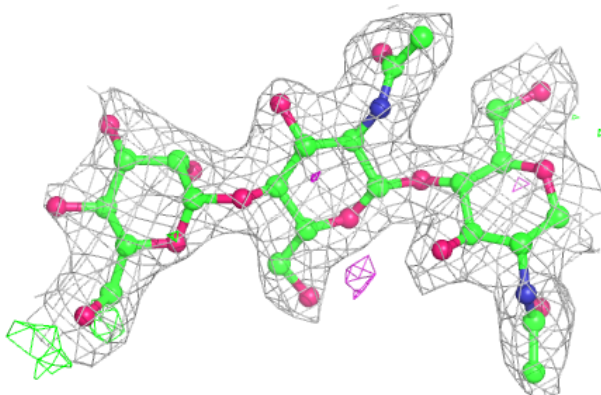


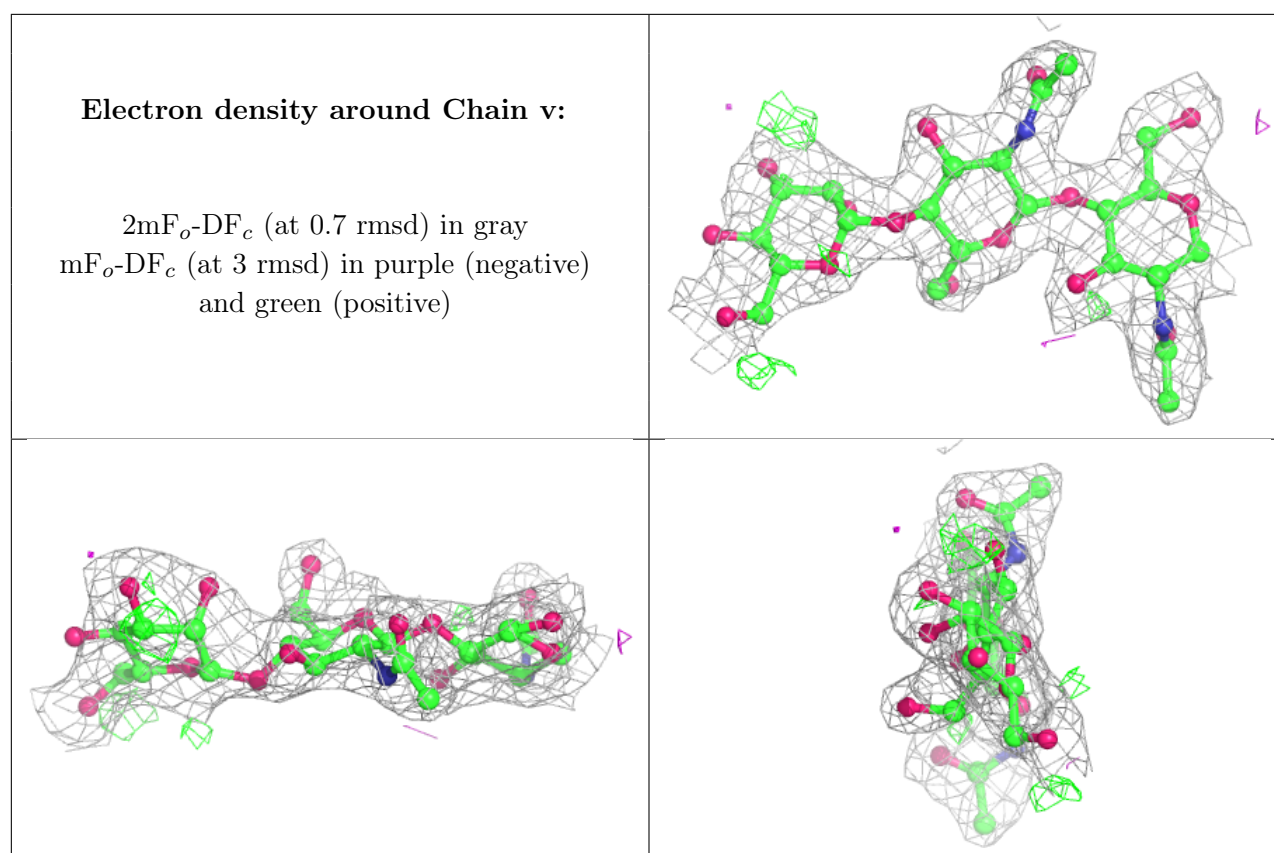
Electron density around Chain n:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain r:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GLC	C	506	12/12	0.75	0.25	71,74,76,77	0
6	NAG	L	1005	14/15	0.76	0.19	48,58,60,60	0
6	NAG	C	501	14/15	0.78	0.32	72,78,84,86	0
6	NAG	E	503	14/15	0.78	0.23	69,74,79,79	0
6	NAG	O	501	14/15	0.79	0.28	71,75,82,84	0
6	NAG	A	503	14/15	0.81	0.27	73,78,82,84	0
6	NAG	O	503	14/15	0.81	0.28	67,72,77,77	0
6	NAG	A	501	14/15	0.81	0.32	62,66,74,76	0
8	GLC	I	506	12/12	0.81	0.26	63,69,70,70	0
6	NAG	I	501	14/15	0.82	0.27	60,67,74,74	0
6	NAG	J	1004	14/15	0.83	0.27	62,68,72,72	0
6	NAG	M	501	14/15	0.83	0.34	67,72,75,76	0
6	NAG	L	1004	14/15	0.83	0.31	75,78,80,81	0
8	GLC	G	506	12/12	0.84	0.18	53,58,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	G	503	14/15	0.84	0.34	70,78,81,81	0
6	NAG	I	503	14/15	0.85	0.25	69,76,81,82	0
6	NAG	F	1003	14/15	0.86	0.19	54,58,63,63	0
8	GLC	P	1002	12/12	0.86	0.20	60,62,63,63	0
6	NAG	G	501	14/15	0.87	0.29	70,73,75,76	0
6	NAG	E	501	14/15	0.87	0.23	71,75,76,77	0
6	NAG	H	1004	14/15	0.87	0.21	54,60,64,65	0
8	GLC	E	506	12/12	0.88	0.21	54,57,57,58	0
6	NAG	B	1004	14/15	0.88	0.19	51,58,62,63	0
6	NAG	D	1003	14/15	0.88	0.19	55,59,63,63	0
8	GLC	L	1002	12/12	0.88	0.19	57,59,61,61	0
6	NAG	N	1003	14/15	0.88	0.19	50,53,57,58	0
6	NAG	C	503	14/15	0.89	0.22	62,66,69,72	0
8	GLC	B	1002	12/12	0.89	0.19	52,56,57,57	0
8	GLC	M	506	12/12	0.90	0.16	50,54,55,55	0
6	NAG	M	504	14/15	0.90	0.15	45,47,50,51	0
6	NAG	H	1003	14/15	0.91	0.16	58,63,64,64	0
6	NAG	C	505	14/15	0.91	0.17	45,55,58,59	0
6	NAG	G	505	14/15	0.91	0.17	42,44,49,49	0
6	NAG	P	1004	14/15	0.91	0.19	57,61,65,66	0
6	NAG	O	505	14/15	0.92	0.20	42,48,52,53	0
6	NAG	G	504	14/15	0.92	0.14	47,50,53,54	0
6	NAG	K	502	14/15	0.93	0.14	43,45,46,46	0
6	NAG	K	503	14/15	0.93	0.15	44,47,49,50	0
6	NAG	E	504	14/15	0.93	0.16	50,54,57,57	0
6	NAG	A	505	14/15	0.93	0.15	36,40,42,43	0
6	NAG	C	504	14/15	0.93	0.15	48,50,53,54	0
6	NAG	I	505	14/15	0.93	0.16	38,41,44,46	0
6	NAG	M	505	14/15	0.93	0.13	40,43,45,47	0
6	NAG	J	1003	14/15	0.93	0.15	53,57,60,63	0
6	NAG	G	502	14/15	0.93	0.13	38,42,44,45	0
6	NAG	K	501	14/15	0.93	0.14	42,45,47,47	0
6	NAG	P	1003	14/15	0.94	0.17	47,50,53,53	0
6	NAG	E	502	14/15	0.94	0.16	36,38,41,41	0
6	NAG	M	503	14/15	0.94	0.16	49,51,53,53	0
6	NAG	D	1002	14/15	0.94	0.14	47,50,51,52	0
6	NAG	A	502	14/15	0.94	0.13	38,40,41,43	0
6	NAG	E	505	14/15	0.94	0.18	43,50,52,53	0
6	NAG	L	1003	14/15	0.94	0.16	46,49,52,52	0
6	NAG	A	504	14/15	0.94	0.12	42,44,46,46	0
6	NAG	O	504	14/15	0.94	0.13	46,49,51,51	0
6	NAG	H	1002	14/15	0.94	0.12	42,44,45,45	0

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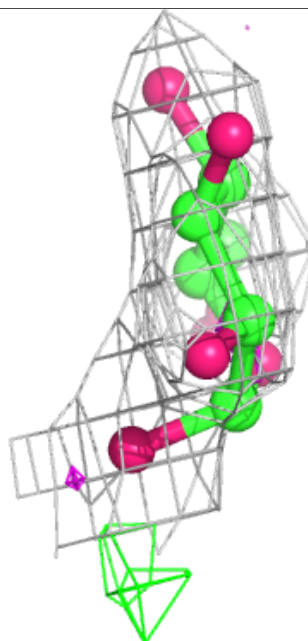
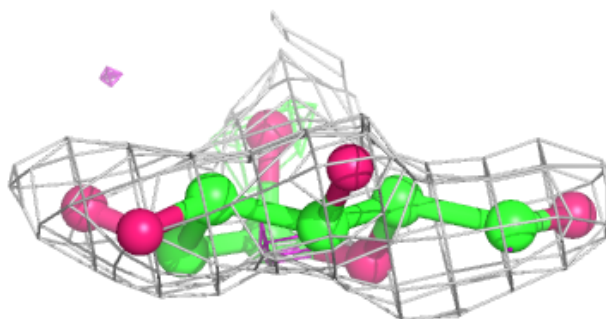
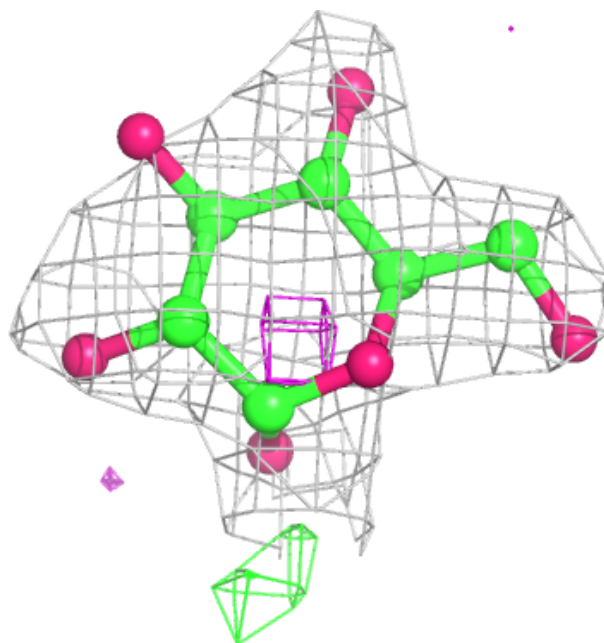
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	F	1002	14/15	0.95	0.12	40,43,44,45	0
6	NAG	N	1002	14/15	0.95	0.12	42,43,44,44	0
6	NAG	B	1003	14/15	0.95	0.13	41,43,44,44	0
6	NAG	C	502	14/15	0.95	0.13	40,42,43,44	0
6	NAG	O	502	14/15	0.95	0.14	40,44,47,48	0
6	NAG	I	504	14/15	0.95	0.13	42,43,45,46	0
6	NAG	J	1002	14/15	0.96	0.13	43,44,45,46	0
6	NAG	I	502	14/15	0.96	0.12	38,39,42,44	0
6	NAG	M	502	14/15	0.97	0.11	34,39,40,42	0
7	NA	F	1001	1/1	0.99	0.15	17,17,17,17	0
7	NA	J	1001	1/1	0.99	0.12	14,14,14,14	0
7	NA	N	1001	1/1	0.99	0.12	12,12,12,12	0
7	NA	P	1001	1/1	0.99	0.12	20,20,20,20	0
7	NA	B	1001	1/1	0.99	0.18	12,12,12,12	0
7	NA	D	1001	1/1	0.99	0.10	16,16,16,16	0
7	NA	H	1001	1/1	1.00	0.12	16,16,16,16	0
7	NA	L	1001	1/1	1.00	0.11	18,18,18,18	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

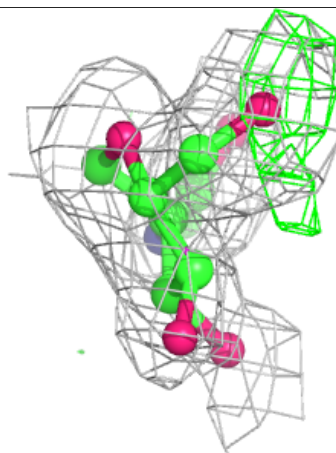
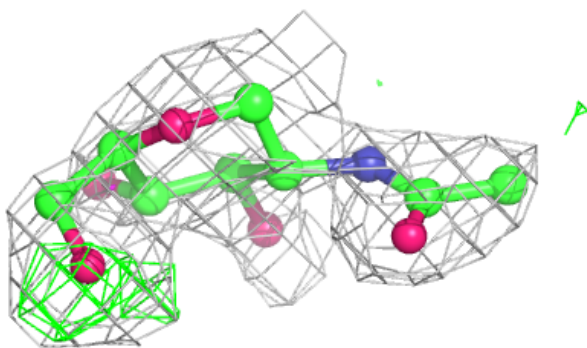
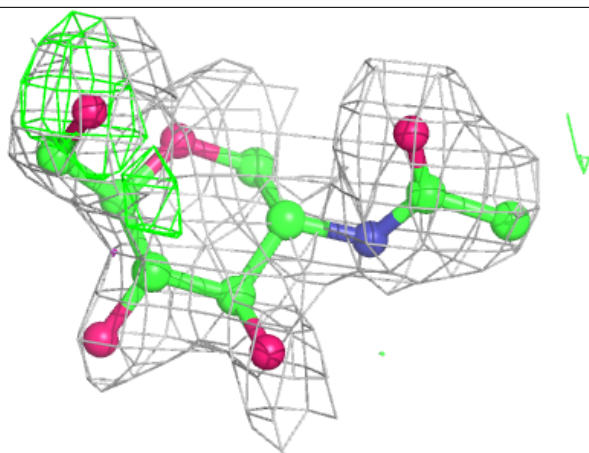
Electron density around GLC C 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

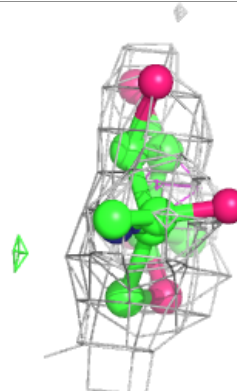
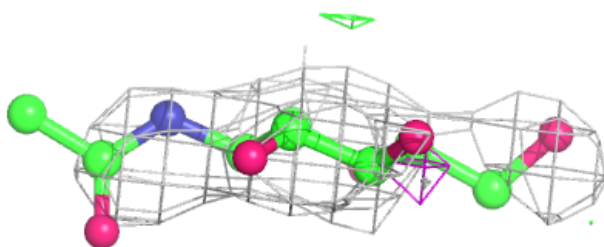
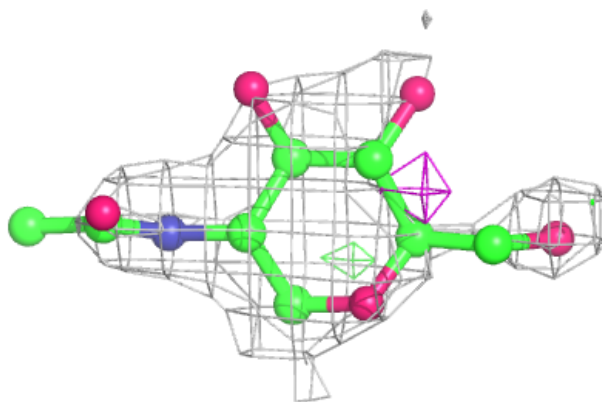


Electron density around NAG L 1005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

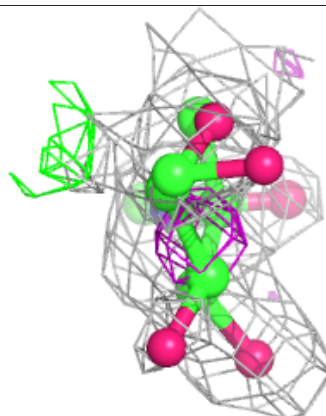
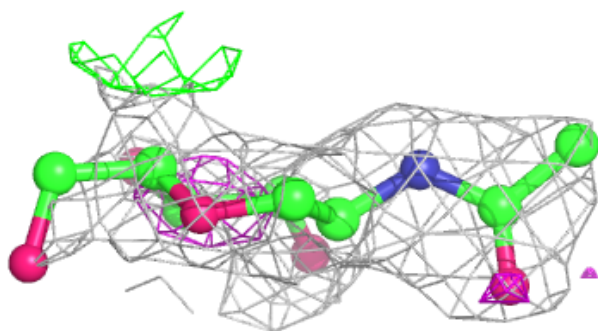
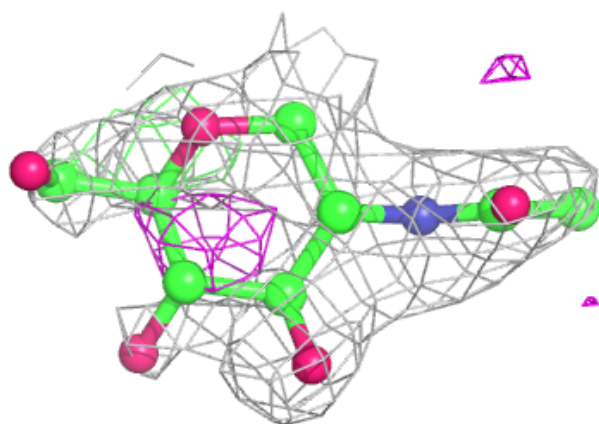
**Electron density around NAG C 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

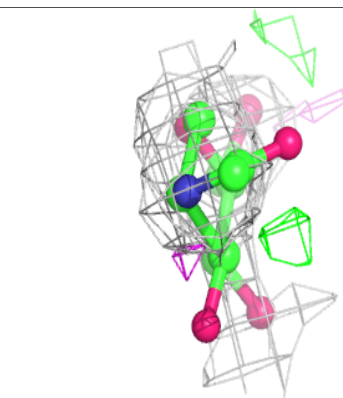
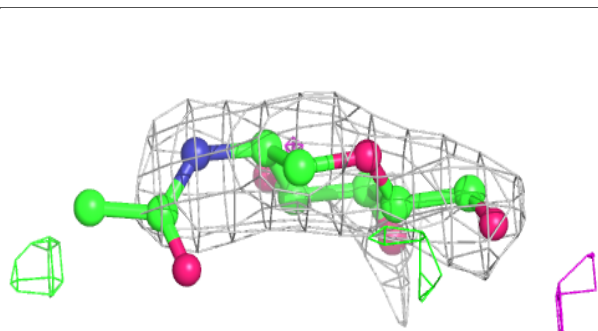
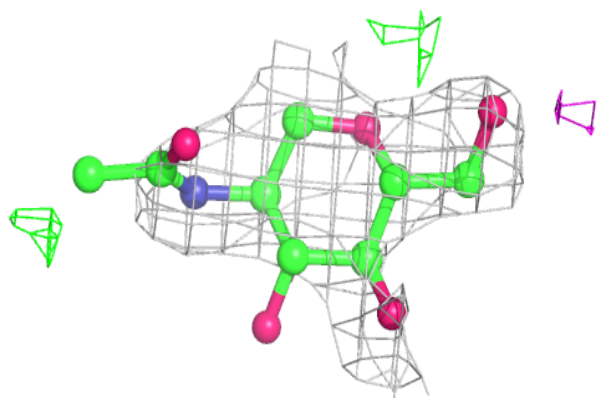


Electron density around NAG E 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

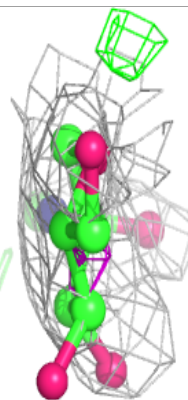
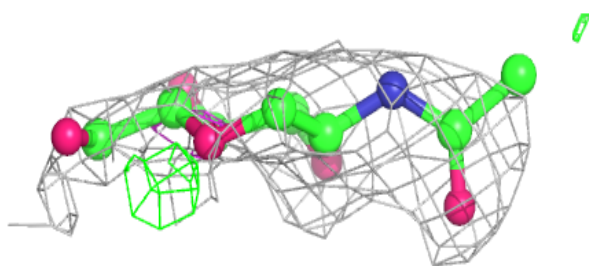
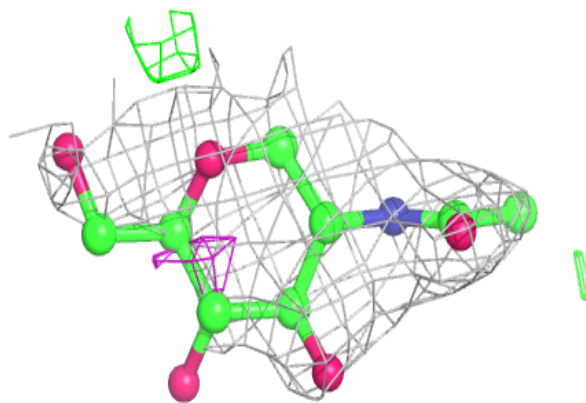
**Electron density around NAG O 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

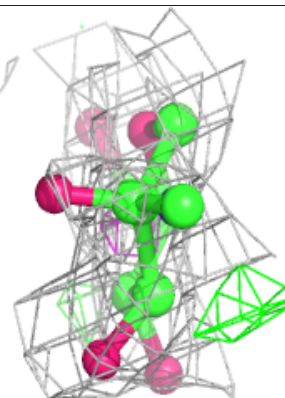
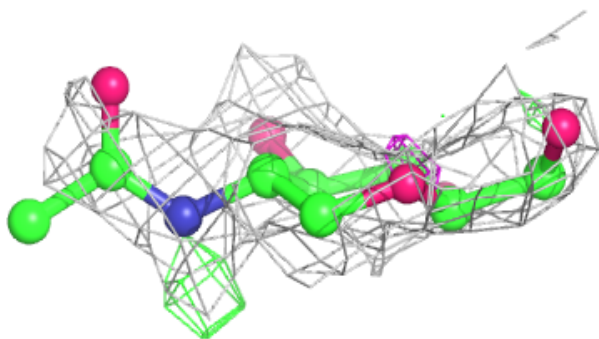
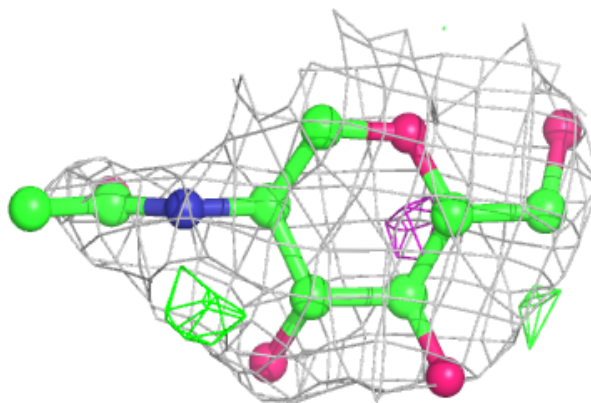


Electron density around NAG A 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

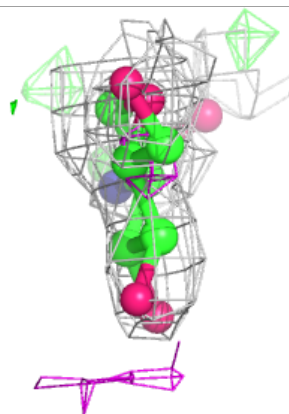
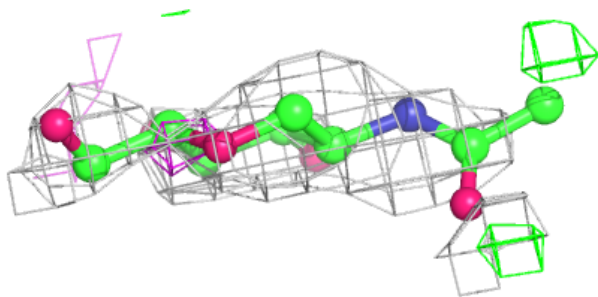
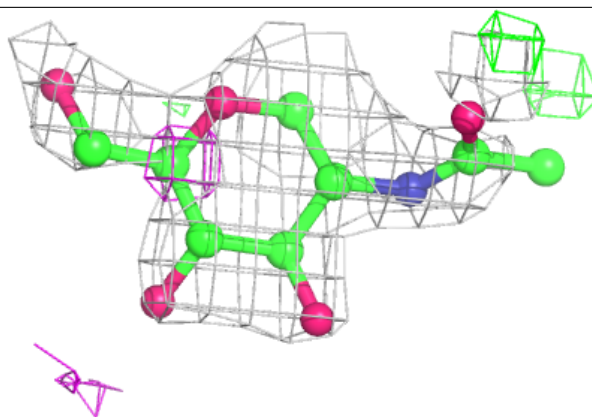
**Electron density around NAG O 503:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



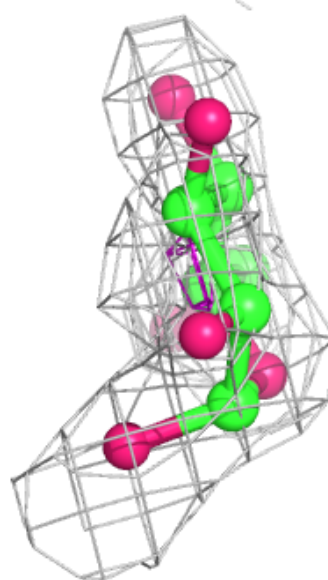
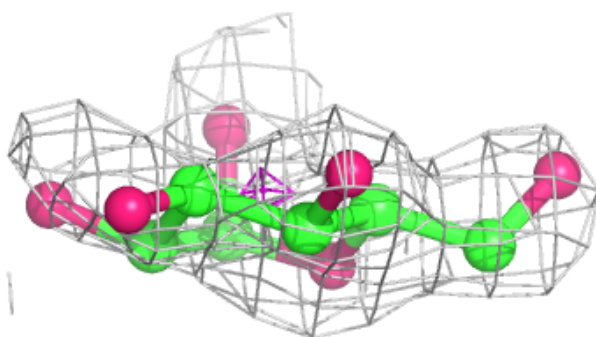
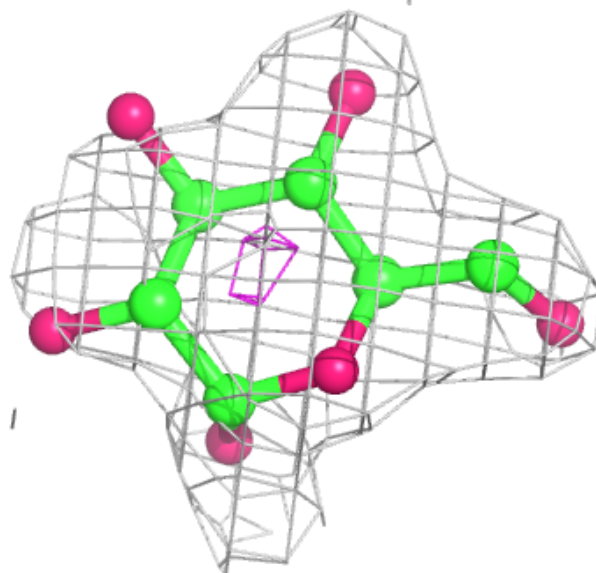
Electron density around NAG A 501:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



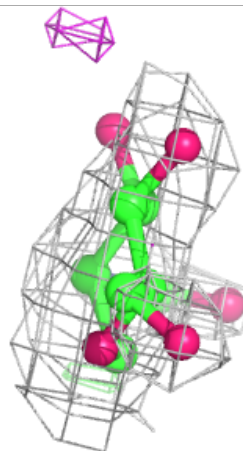
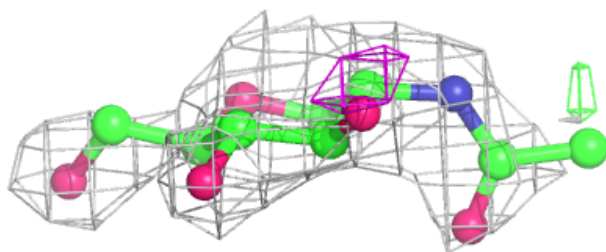
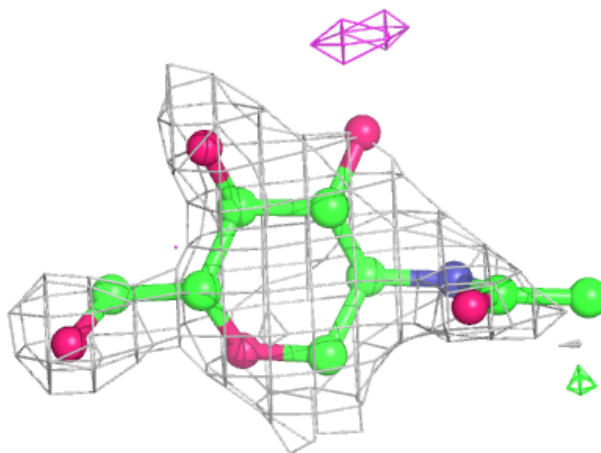
Electron density around GLC I 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



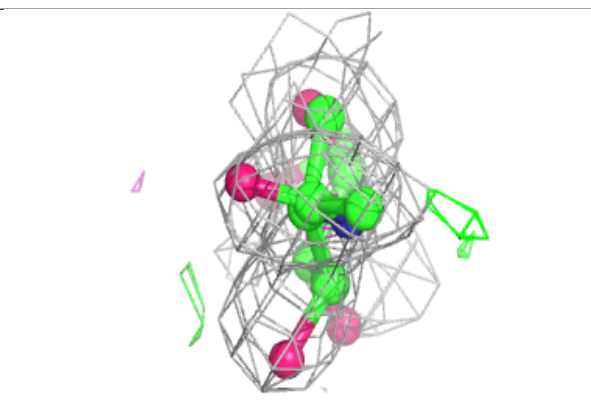
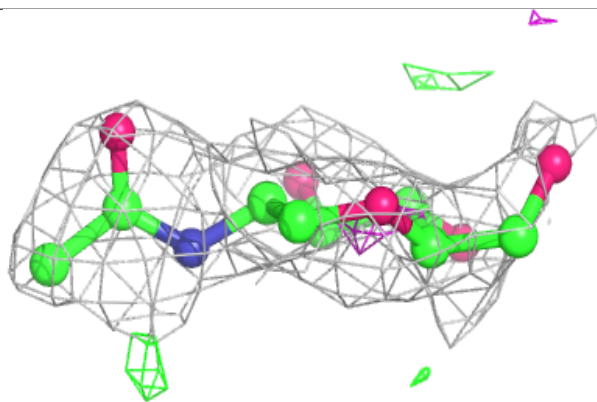
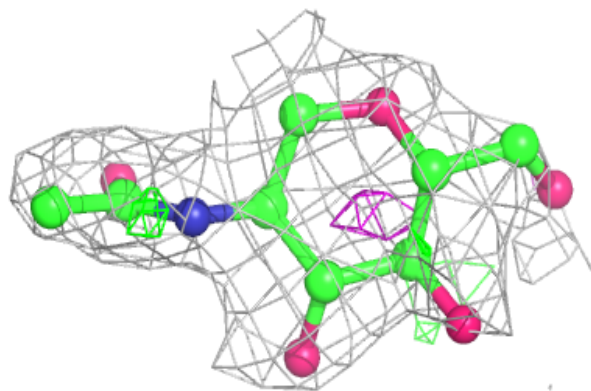
Electron density around NAG I 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

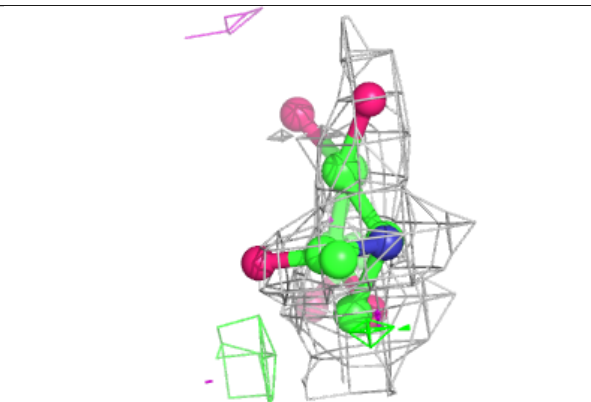
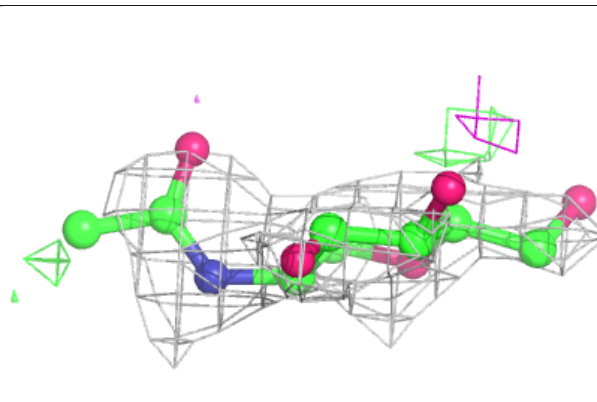
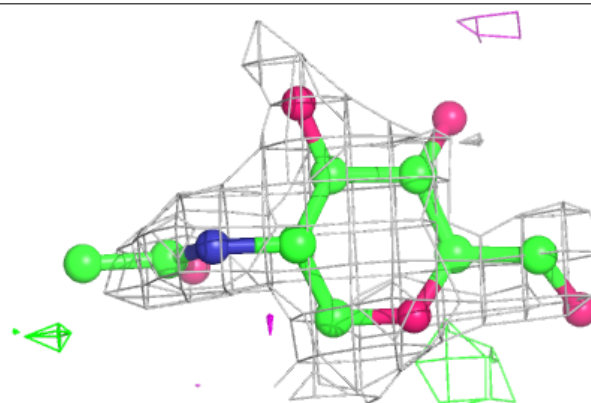


Electron density around NAG J 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

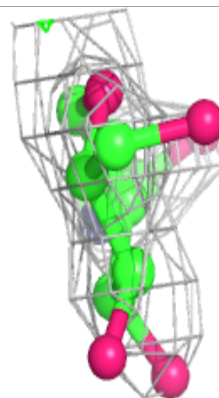
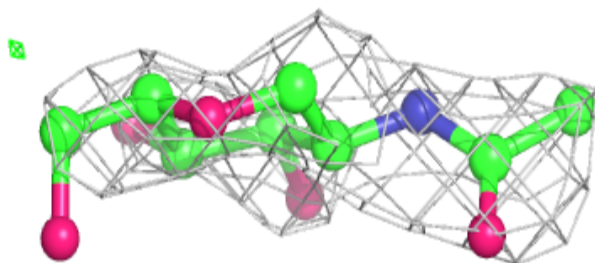
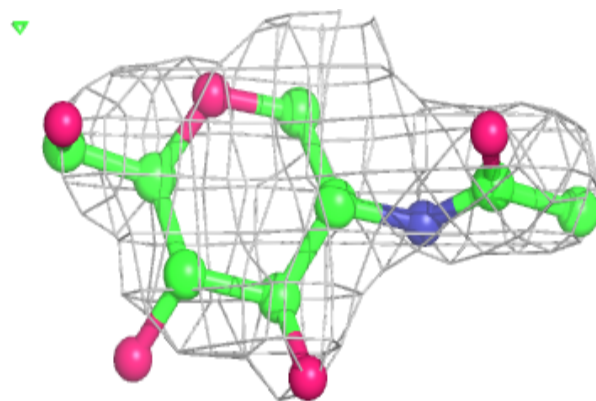
**Electron density around NAG M 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



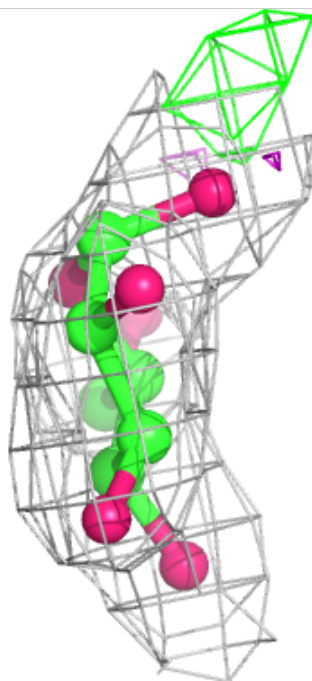
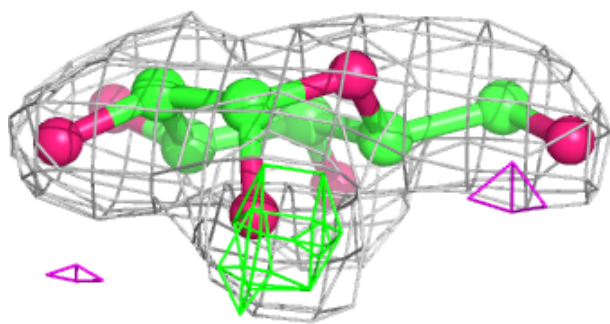
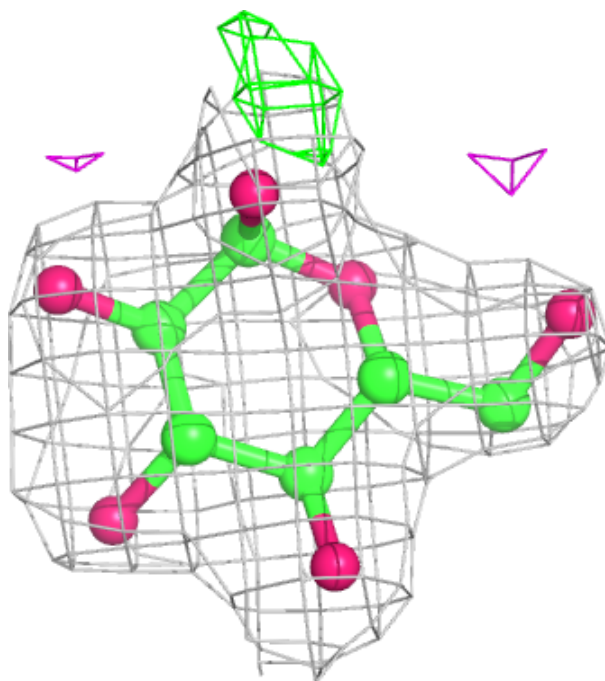
Electron density around NAG L 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



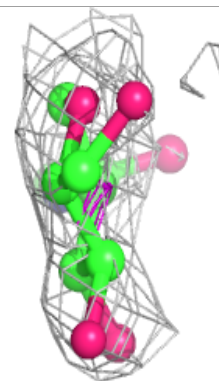
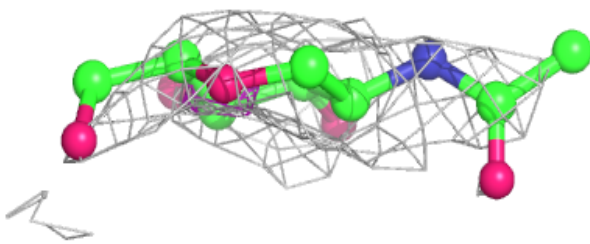
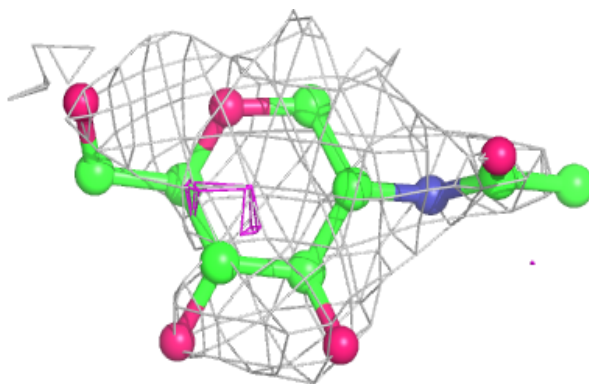
Electron density around GLC G 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

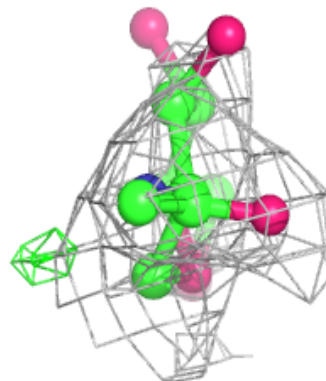
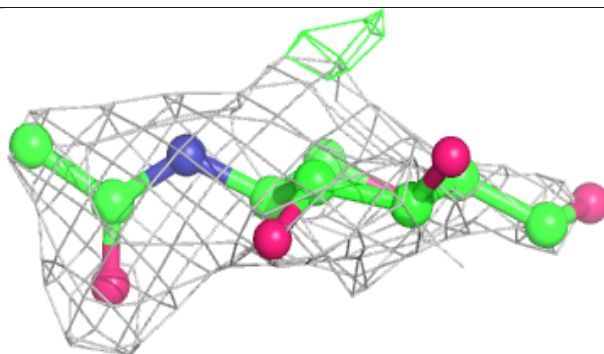
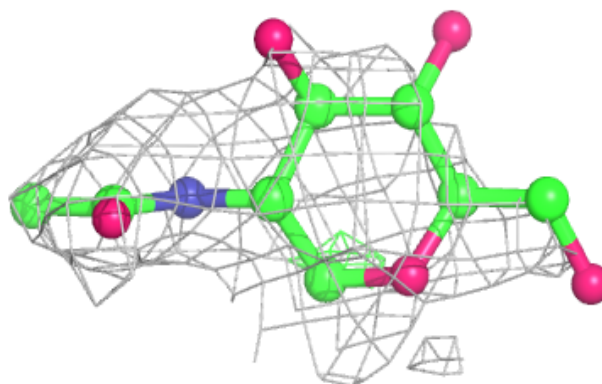


Electron density around NAG G 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

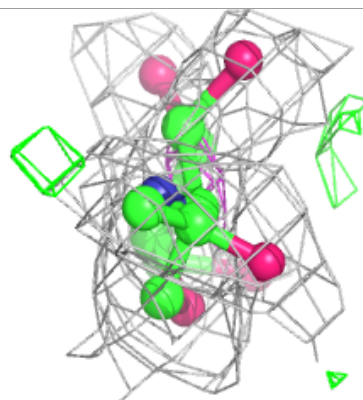
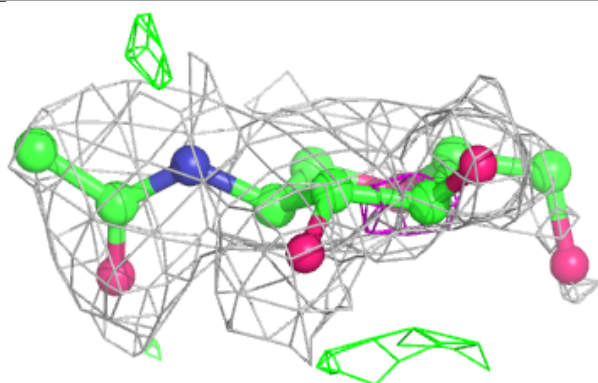
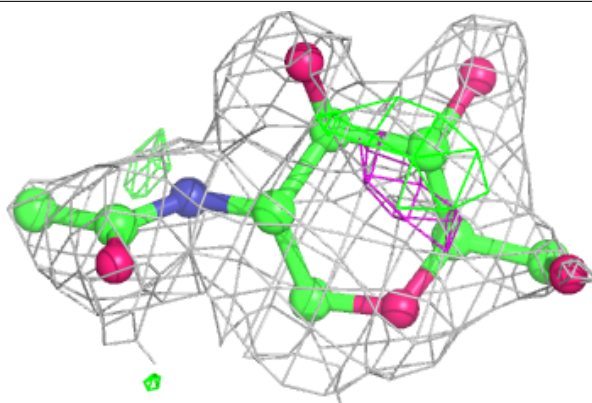
**Electron density around NAG I 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



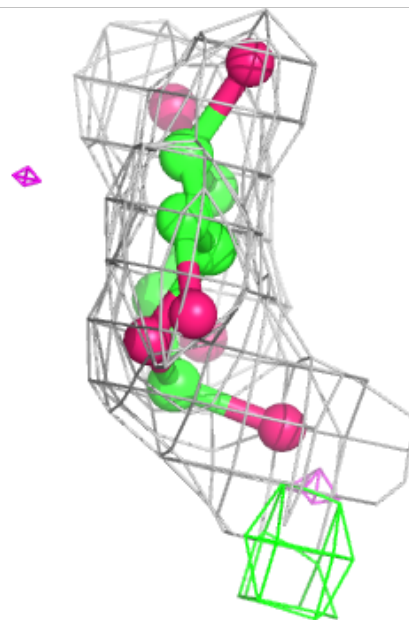
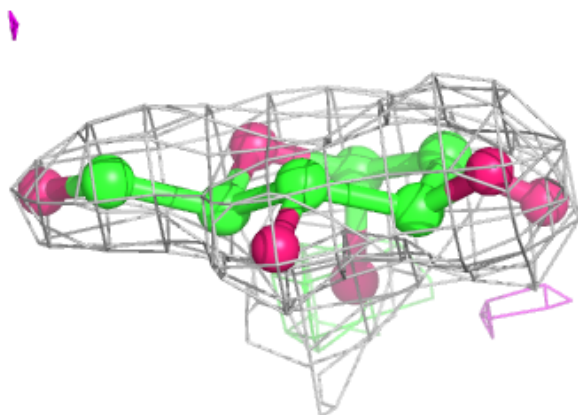
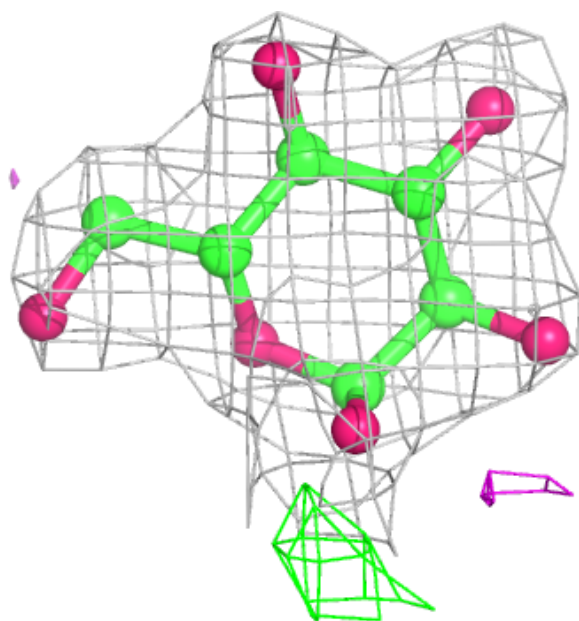
Electron density around NAG F 1003:

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and green (positive)



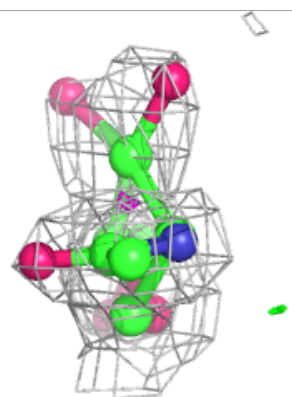
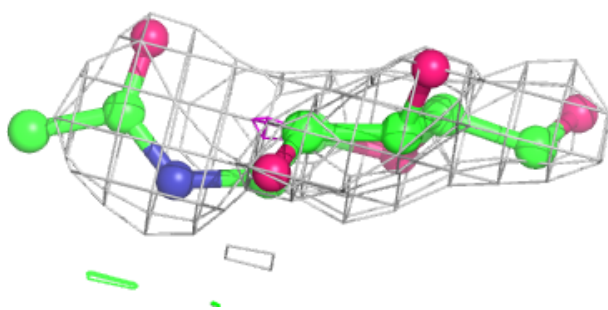
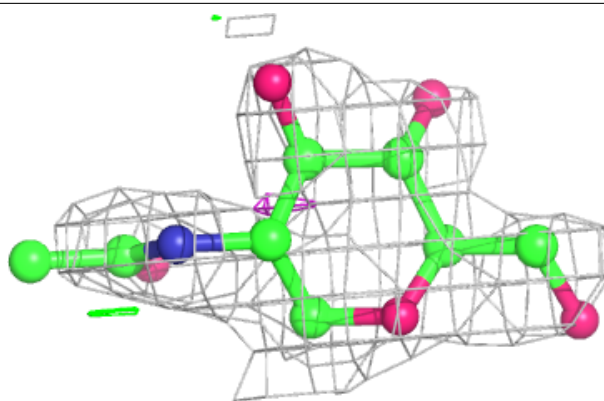
Electron density around GLC P 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

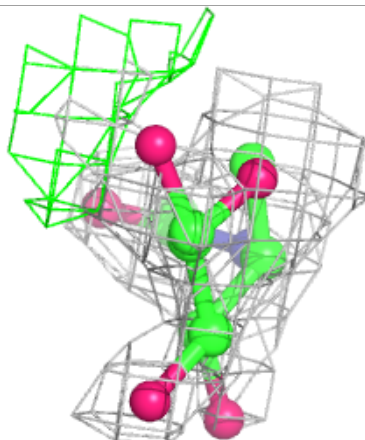
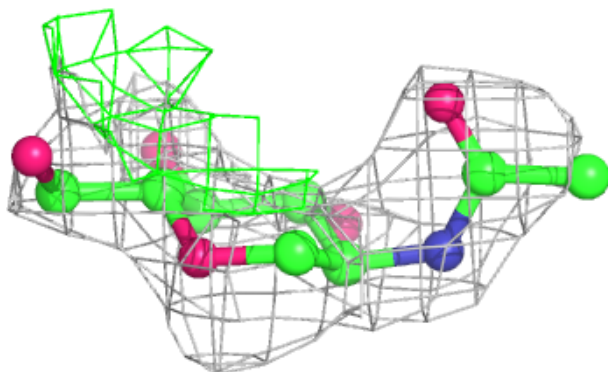
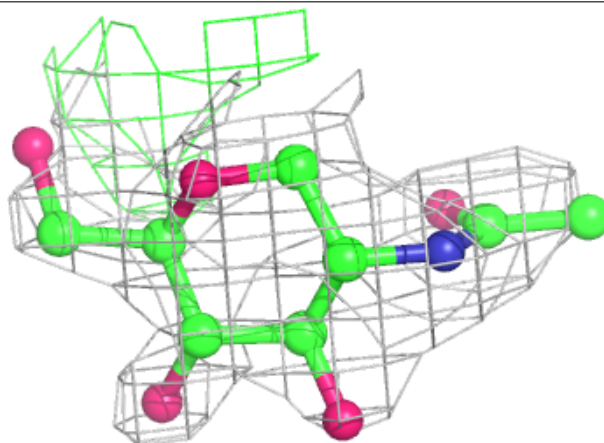


Electron density around NAG G 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

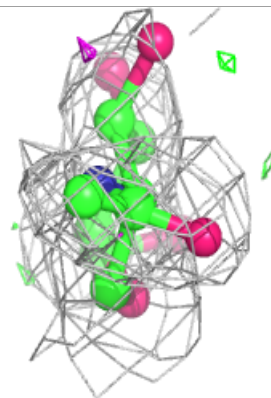
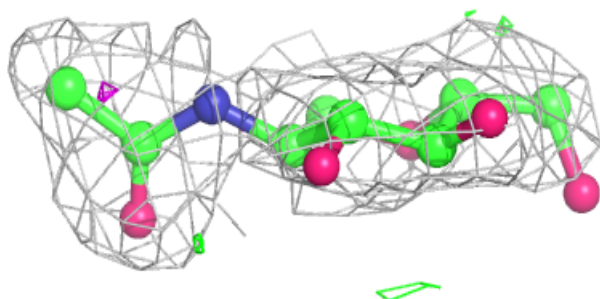
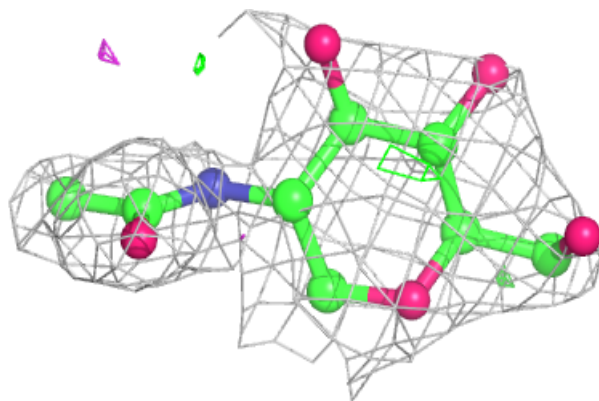
**Electron density around NAG E 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



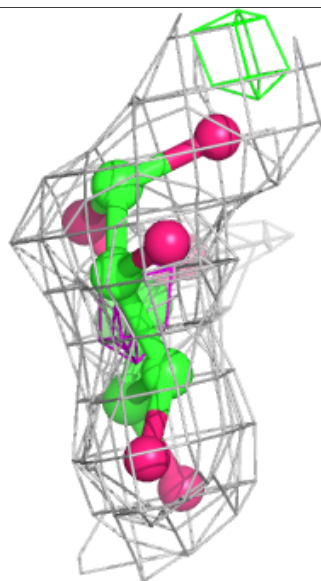
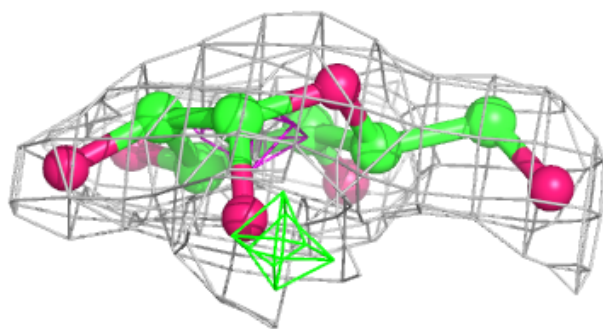
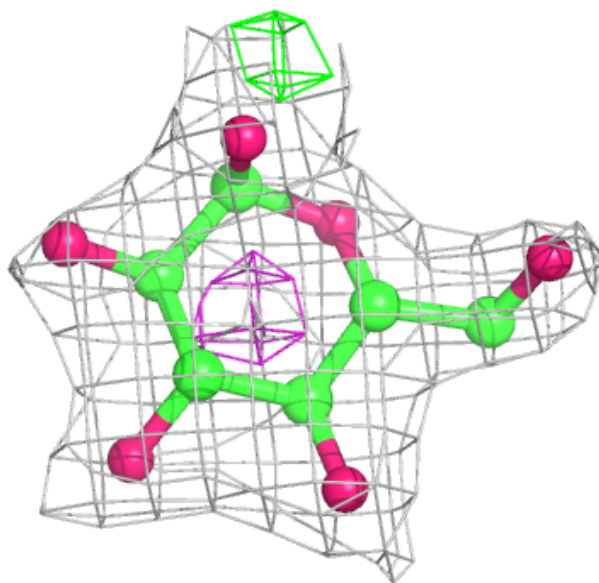
Electron density around NAG H 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



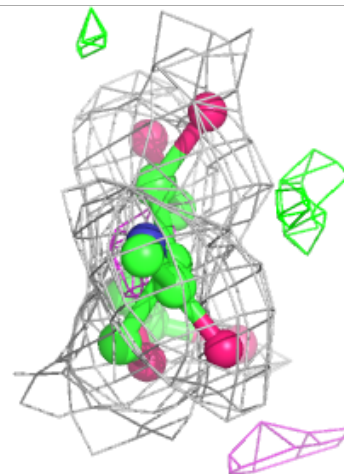
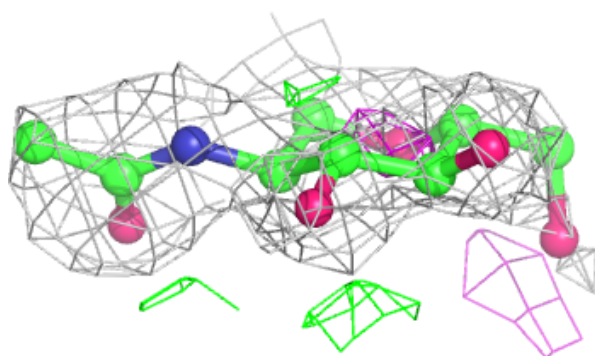
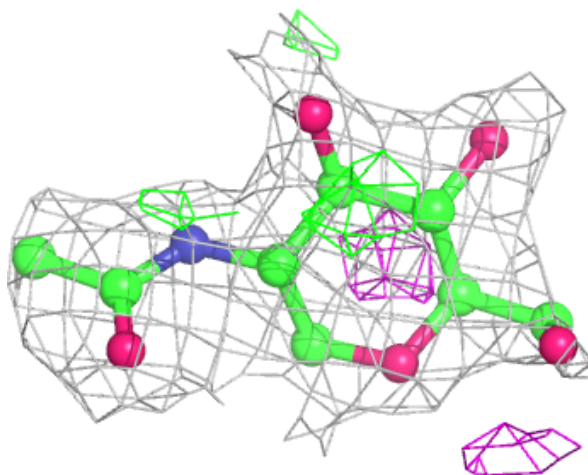
Electron density around GLC E 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



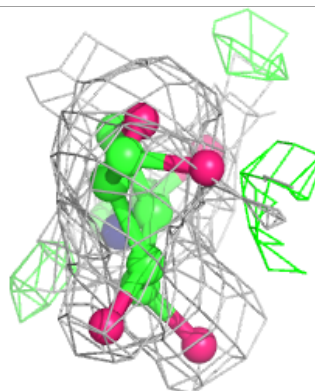
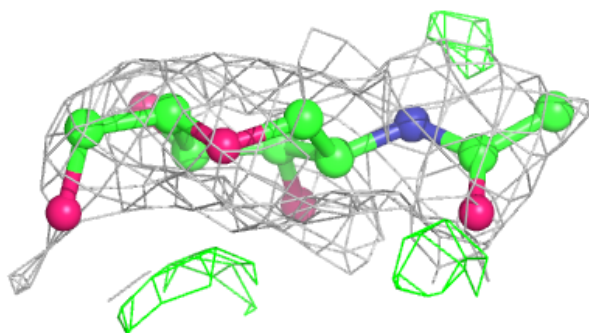
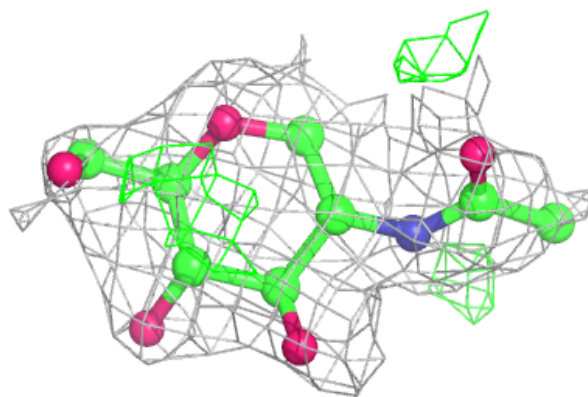
Electron density around NAG B 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



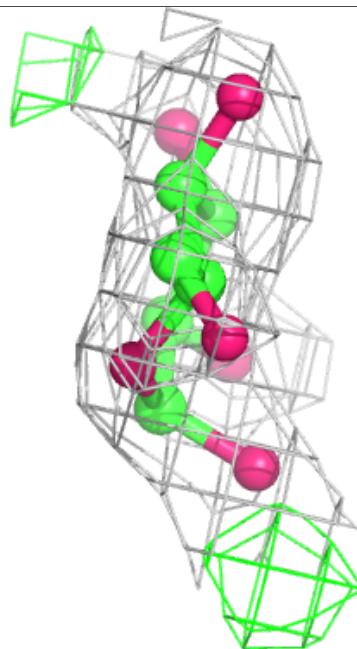
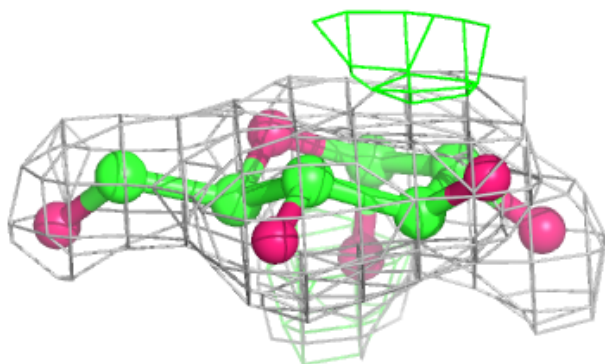
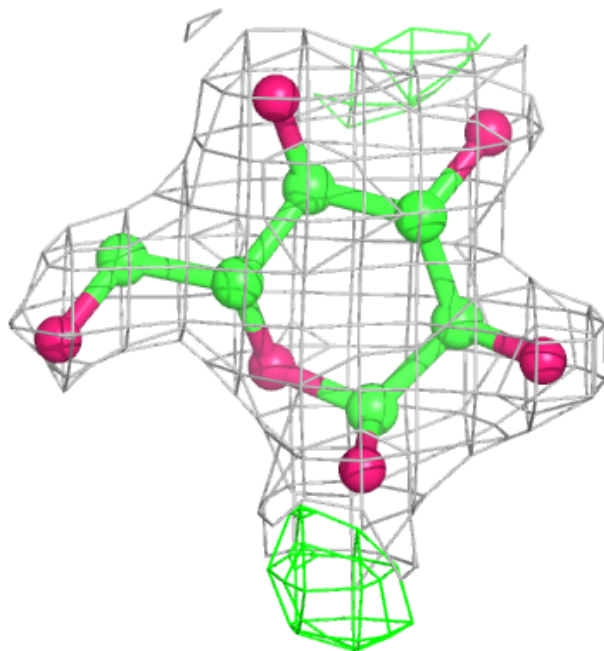
Electron density around NAG D 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



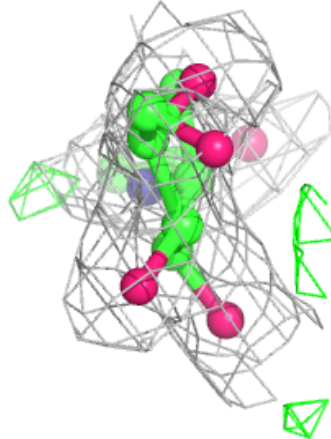
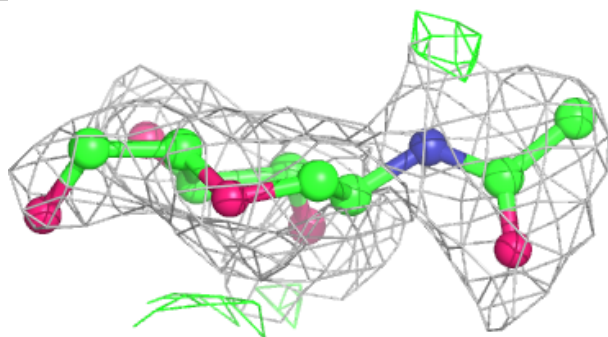
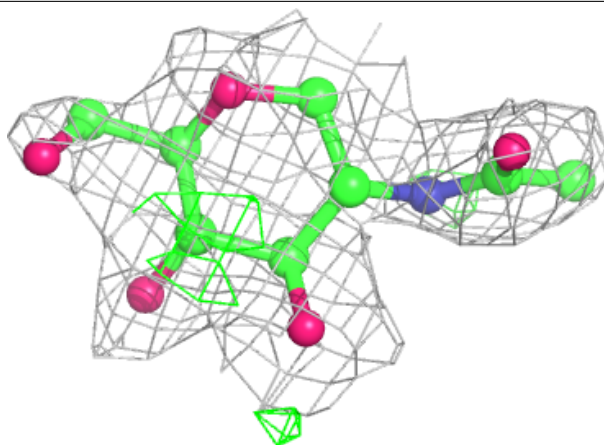
Electron density around GLC L 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



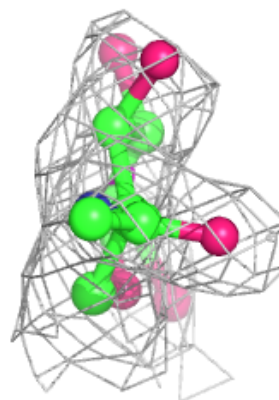
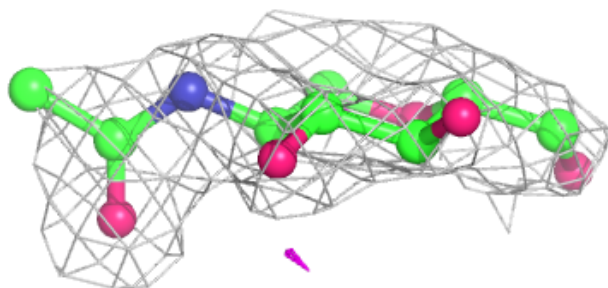
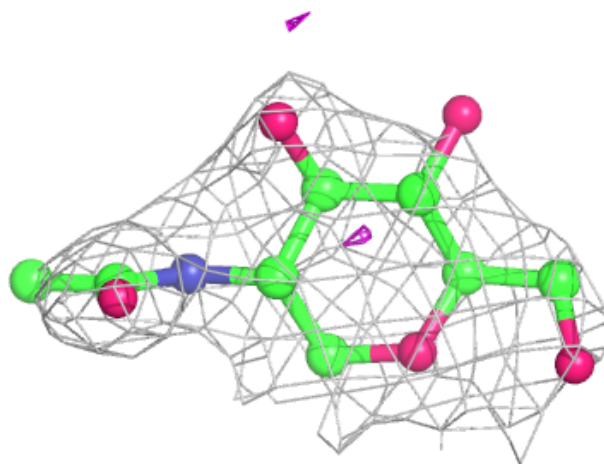
Electron density around NAG N 1003:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



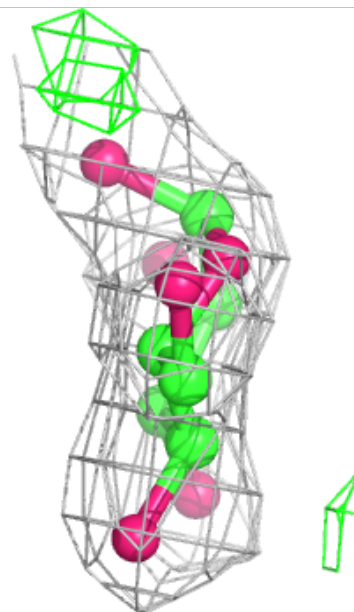
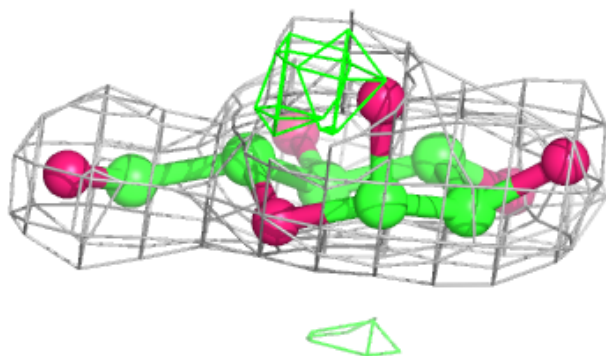
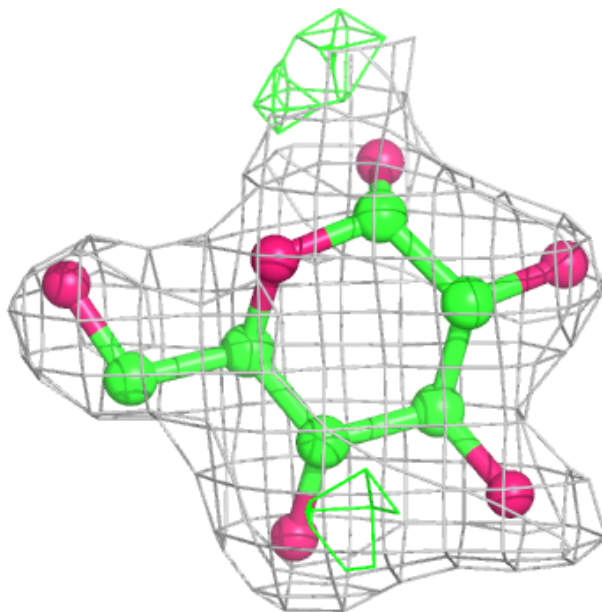
Electron density around NAG C 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



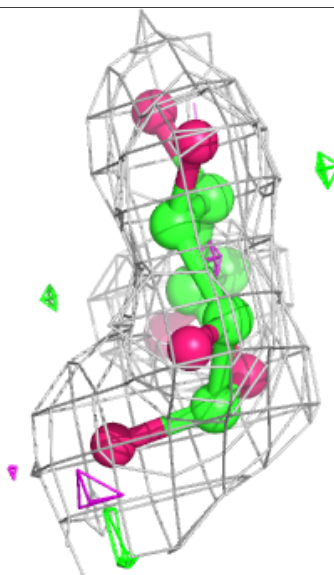
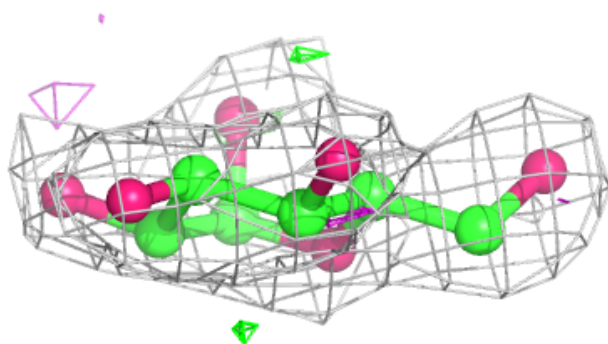
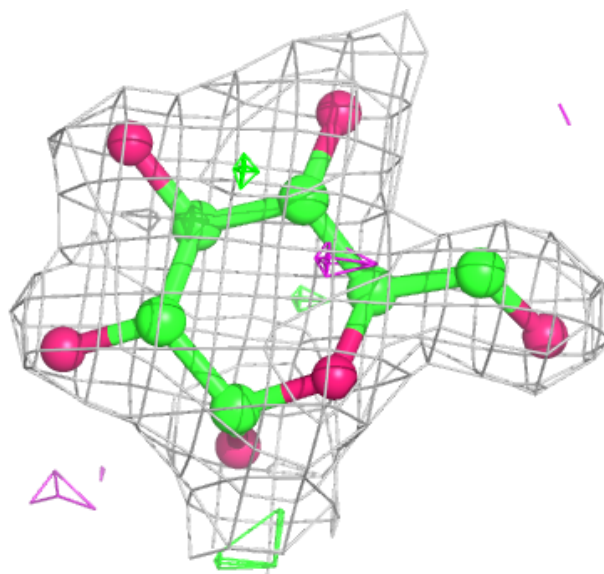
Electron density around GLC B 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



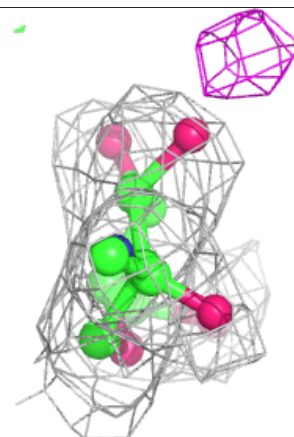
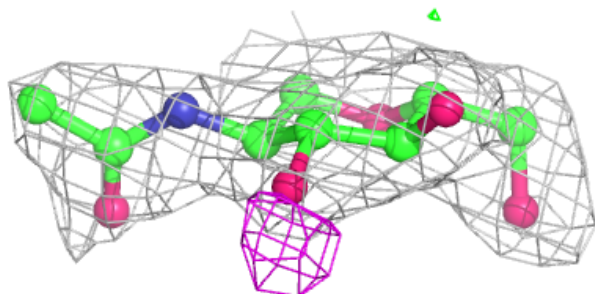
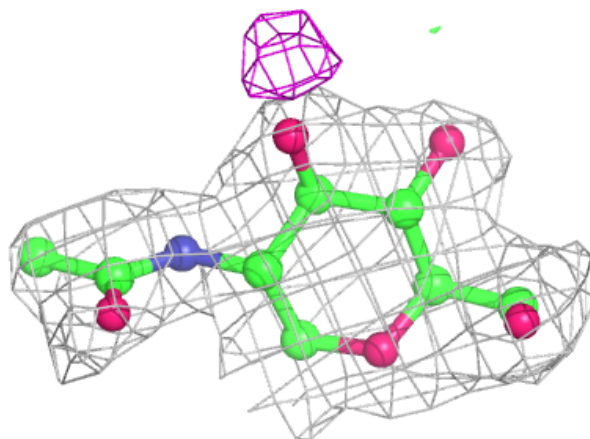
Electron density around GLC M 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

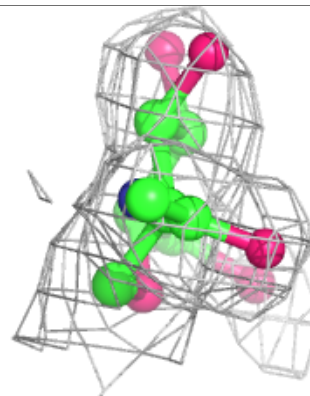
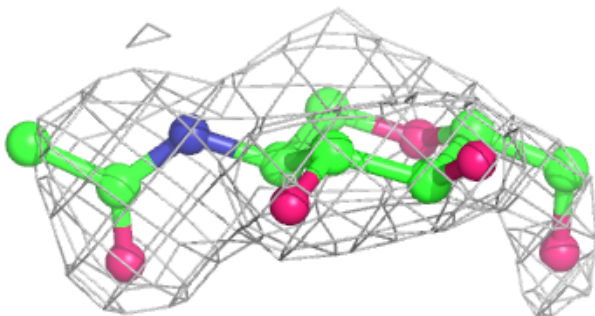
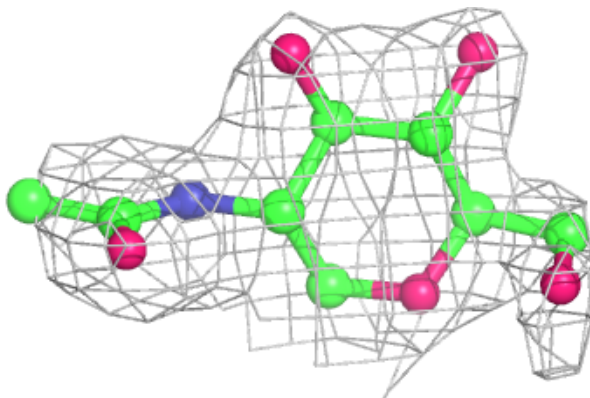


Electron density around NAG M 504:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

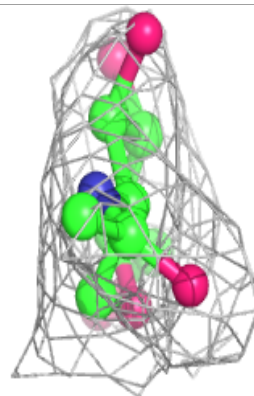
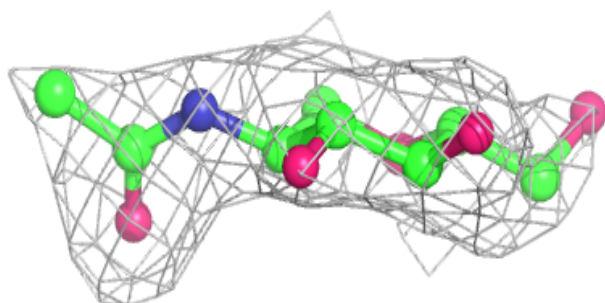
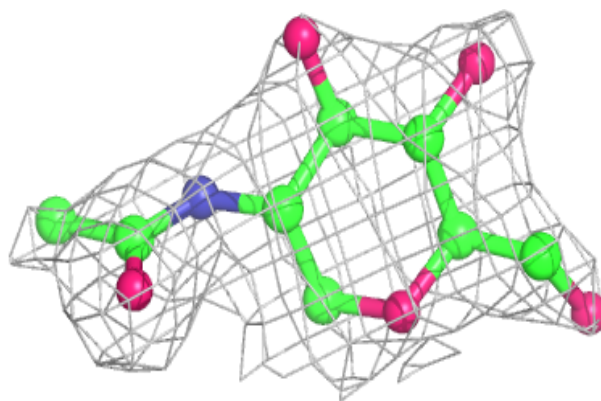
**Electron density around NAG H 1003:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

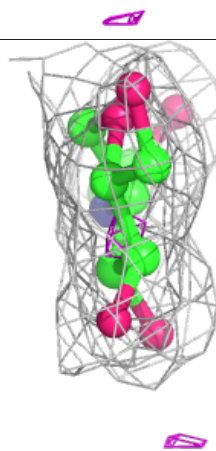
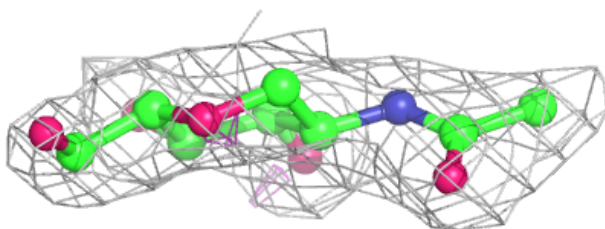
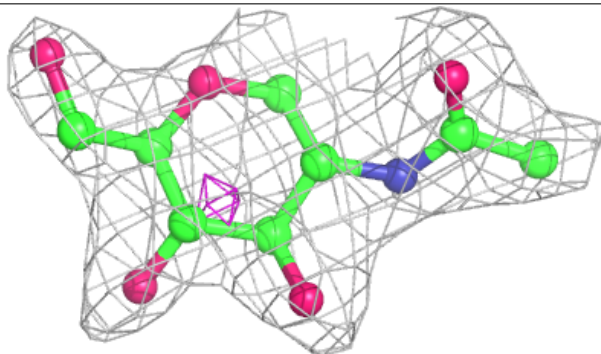


Electron density around NAG C 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

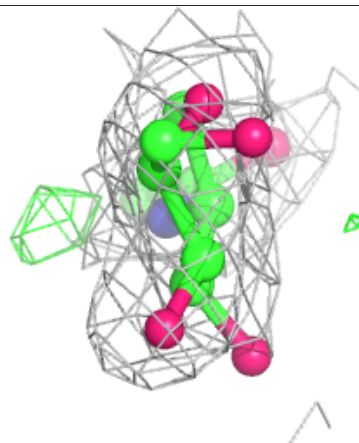
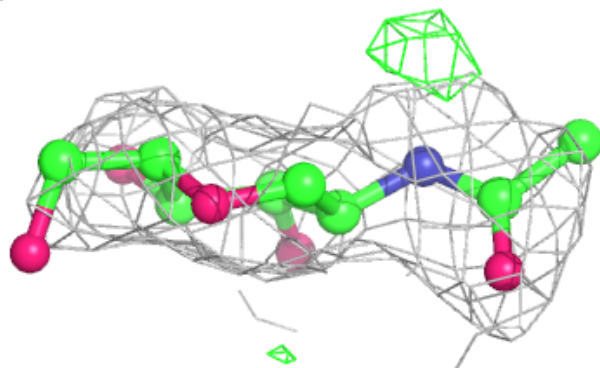
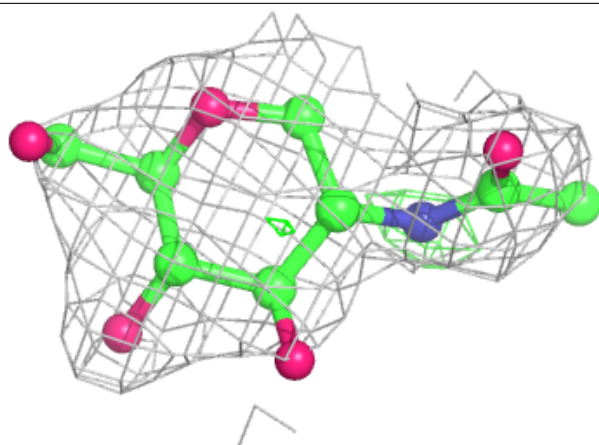
**Electron density around NAG G 505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



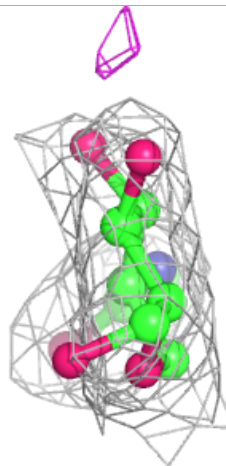
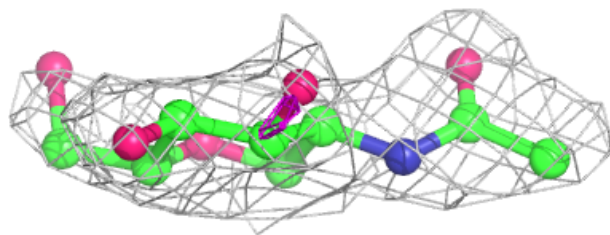
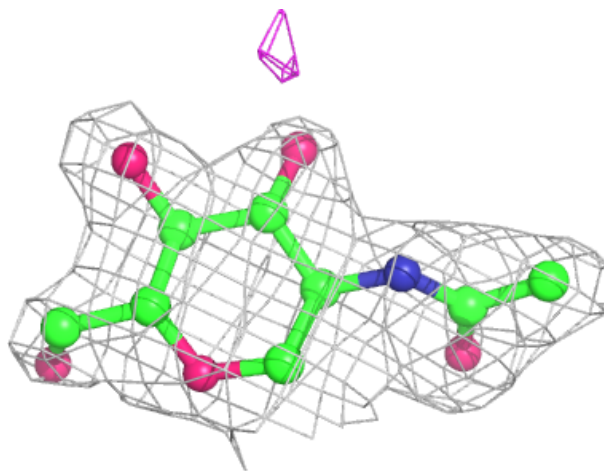
Electron density around NAG P 1004:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



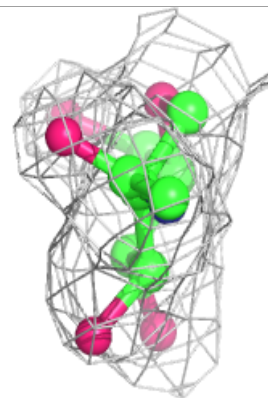
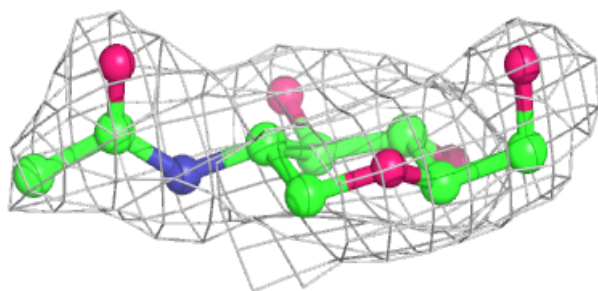
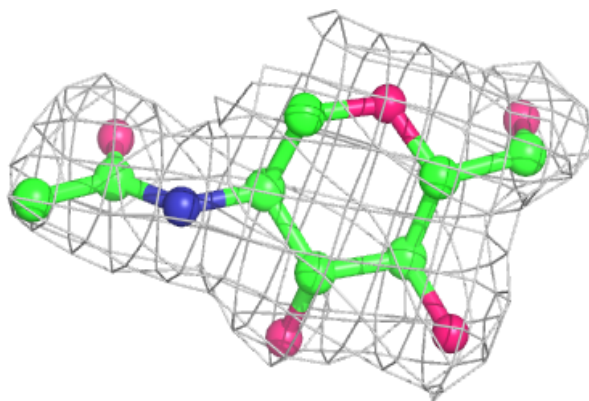
Electron density around NAG O 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

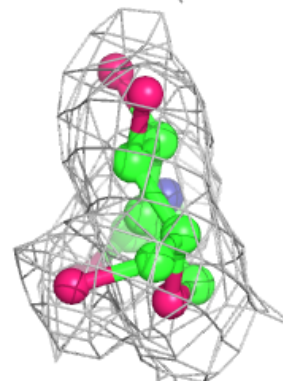
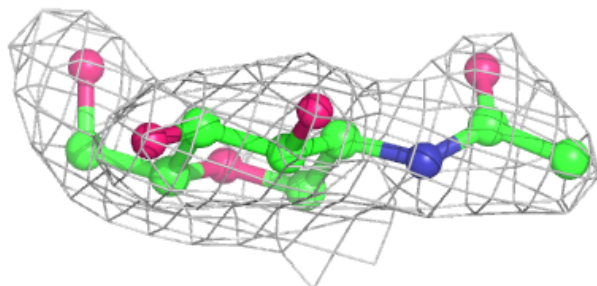
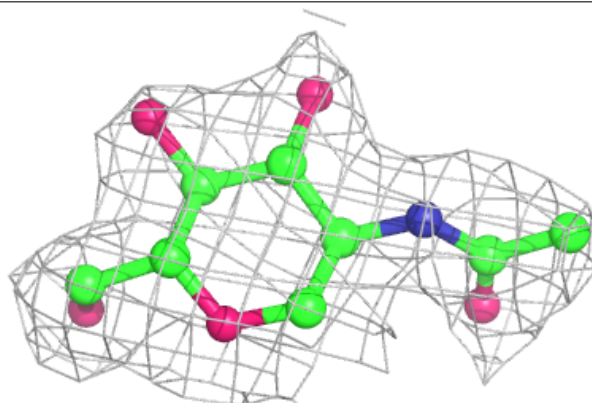


Electron density around NAG G 504:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

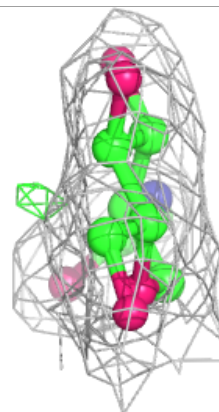
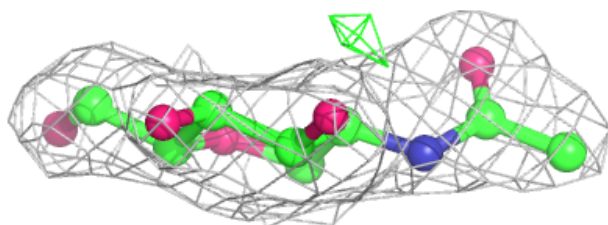
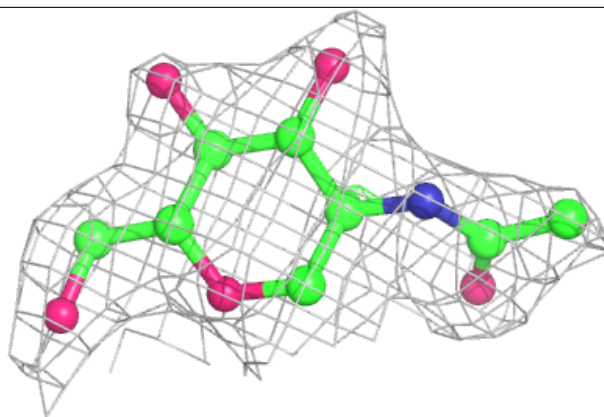
**Electron density around NAG K 502:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

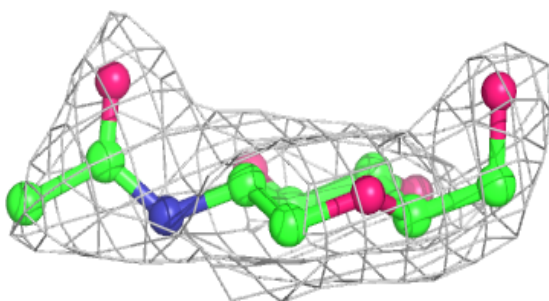
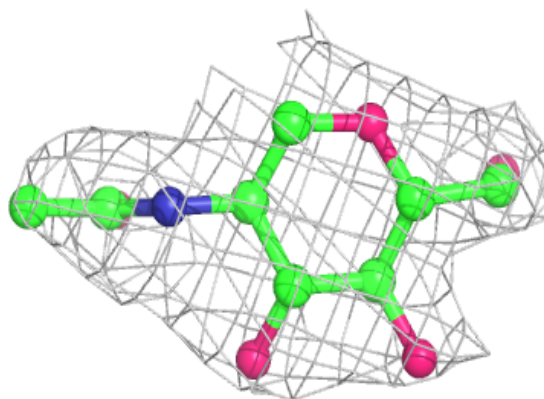


Electron density around NAG K 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

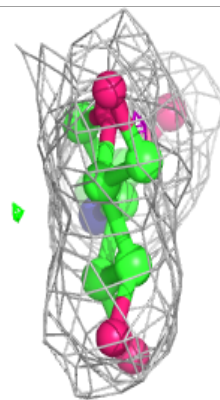
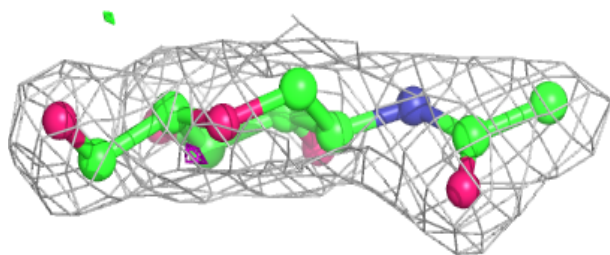
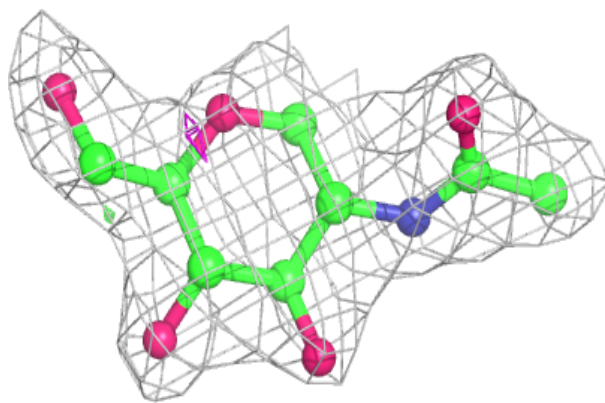
**Electron density around NAG E 504:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



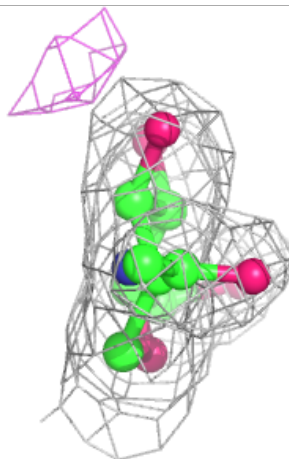
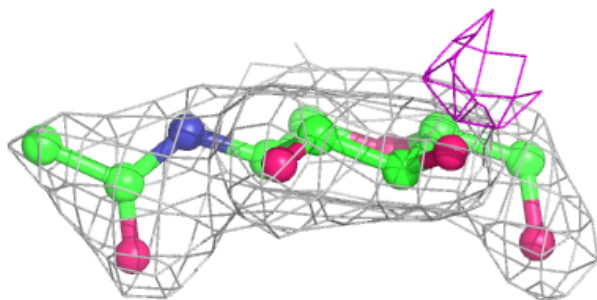
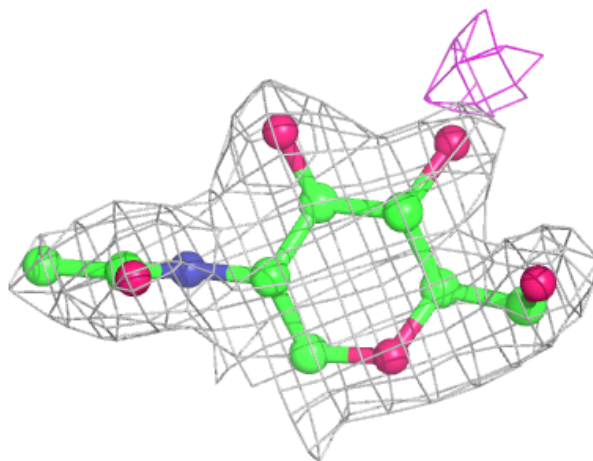
Electron density around NAG A 505:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



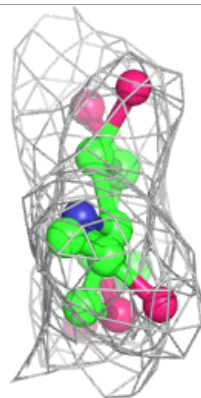
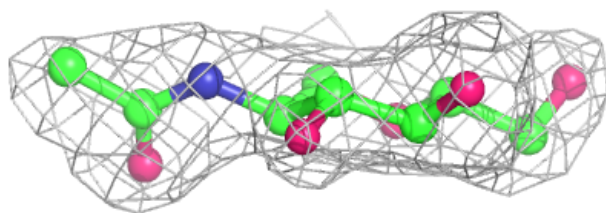
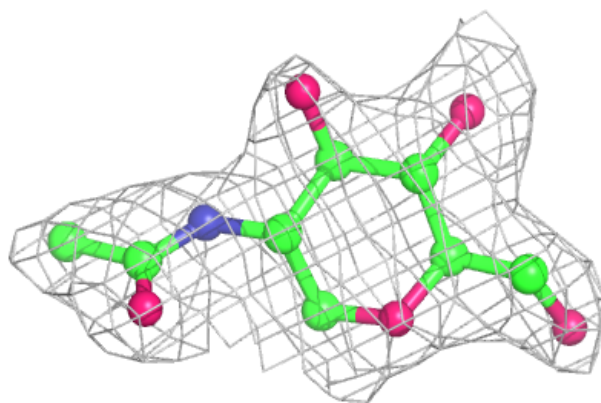
Electron density around NAG C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



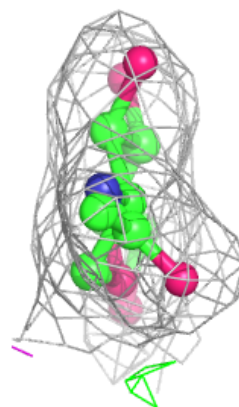
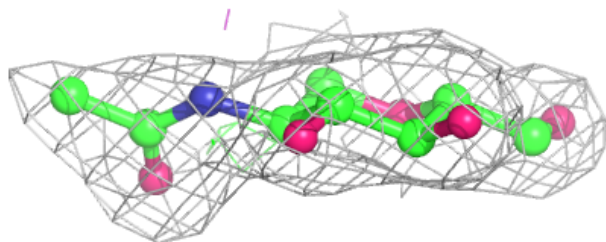
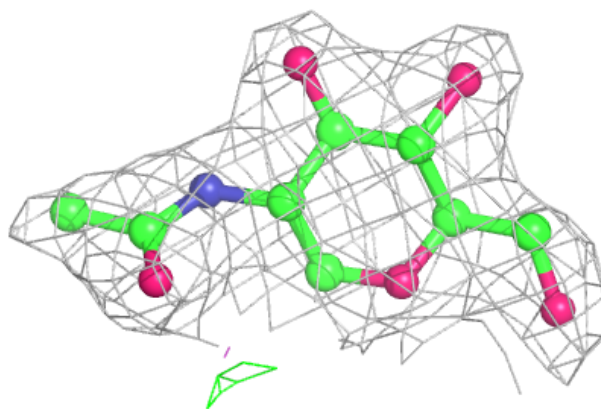
Electron density around NAG I 505:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



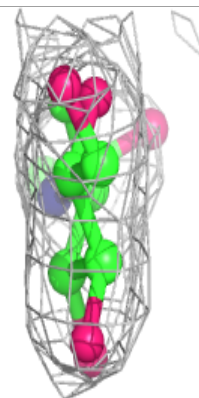
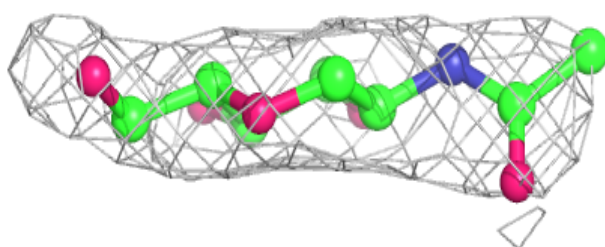
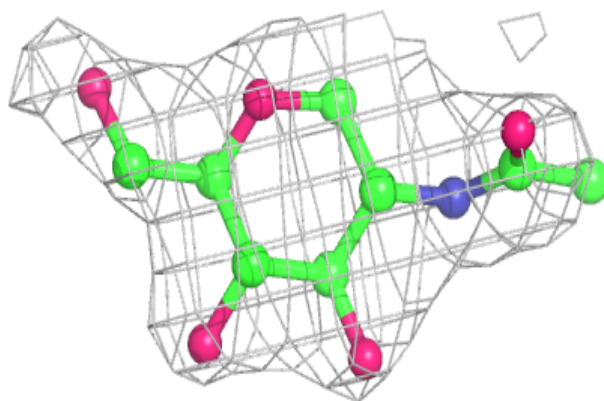
Electron density around NAG M 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

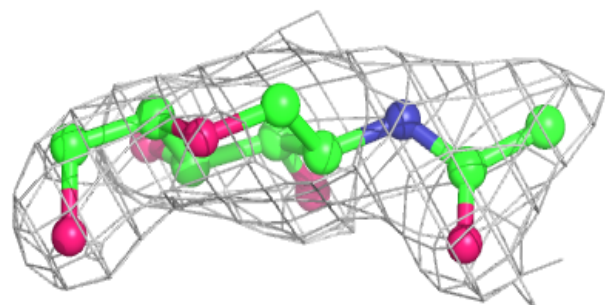
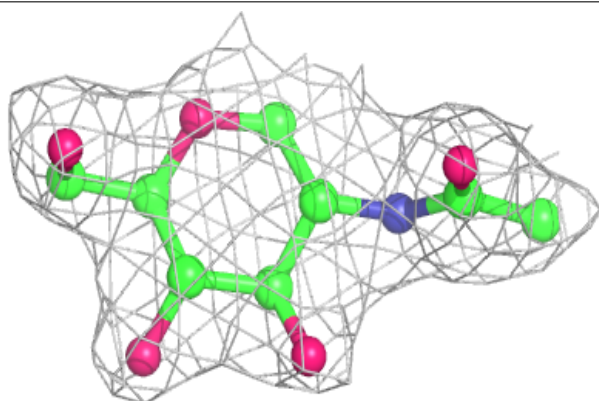


Electron density around NAG J 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

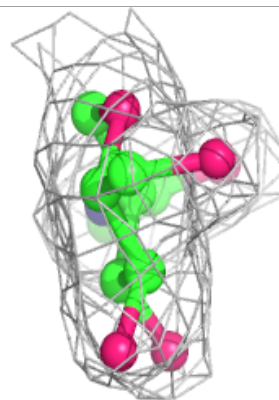
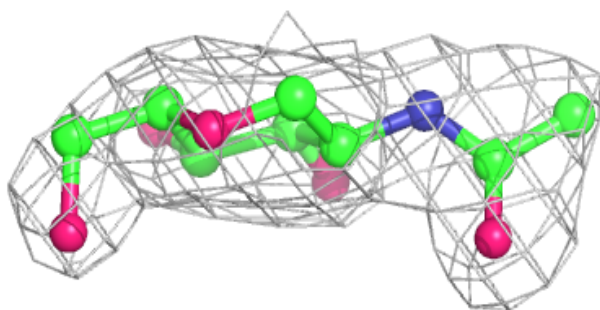
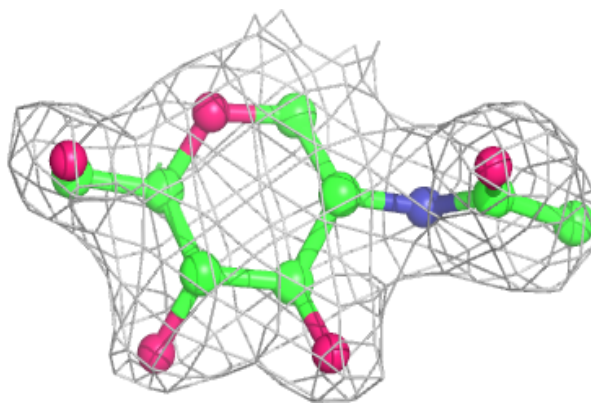
**Electron density around NAG G 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

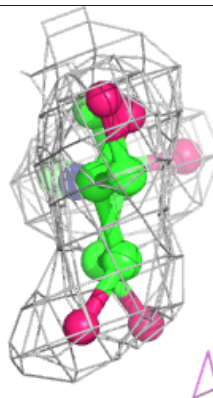
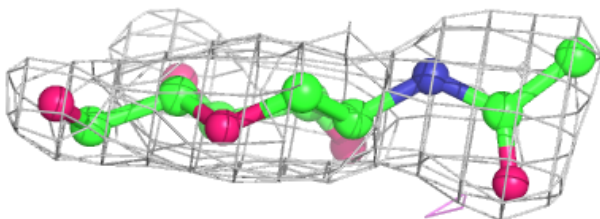
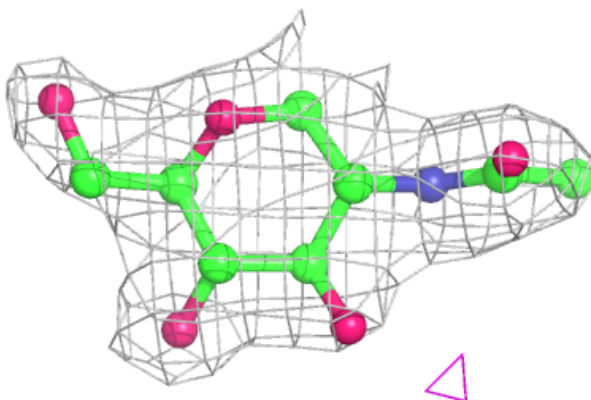


Electron density around NAG K 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

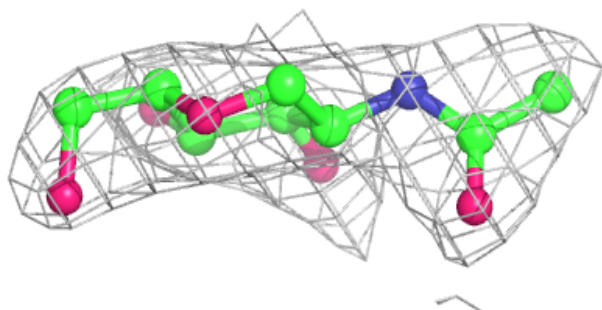
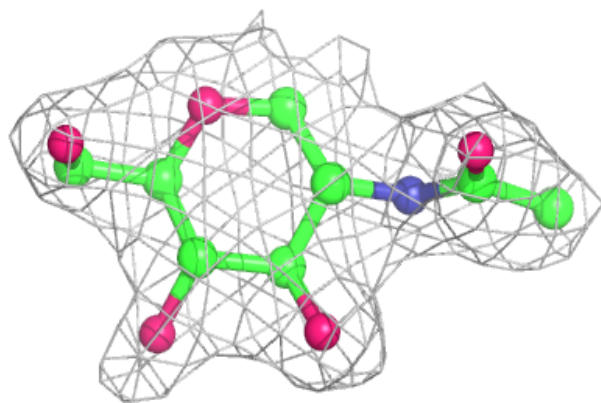
**Electron density around NAG P 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

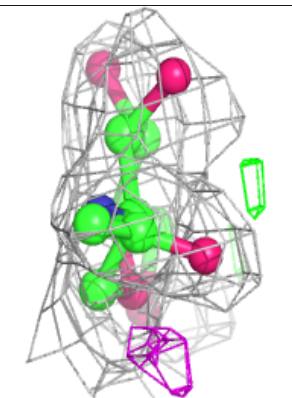
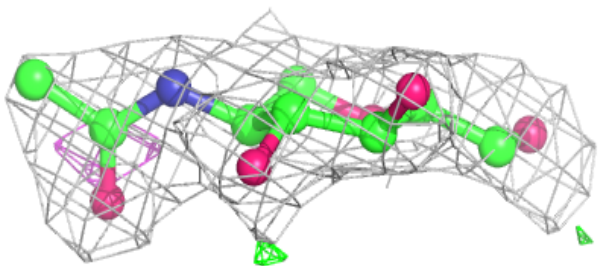
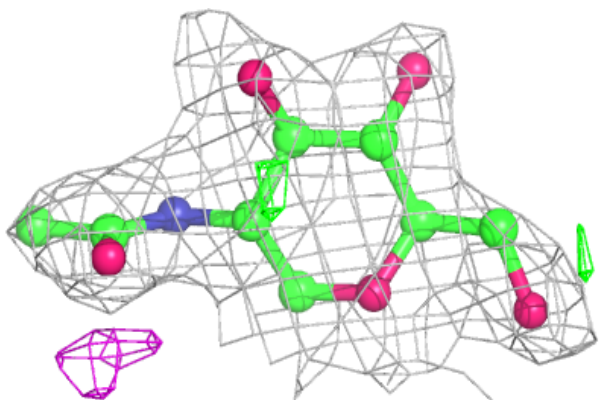


Electron density around NAG E 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

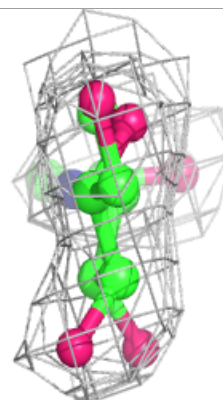
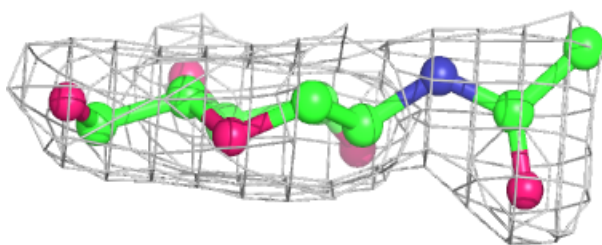
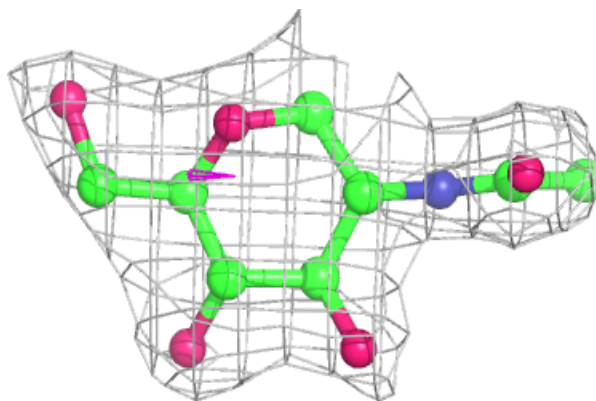
**Electron density around NAG M 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

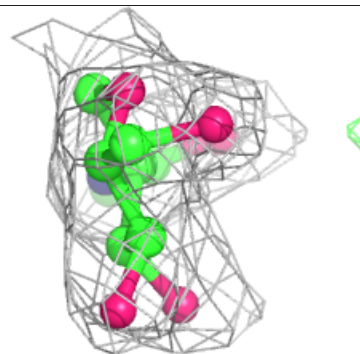
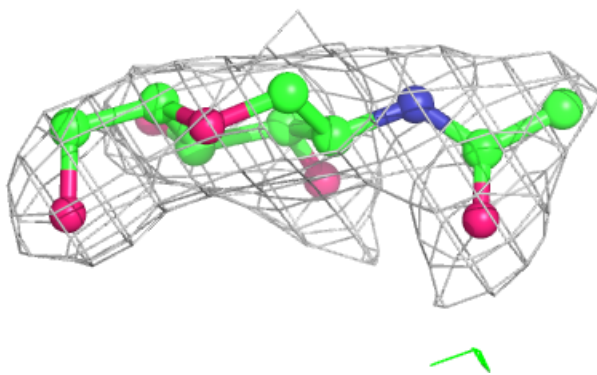
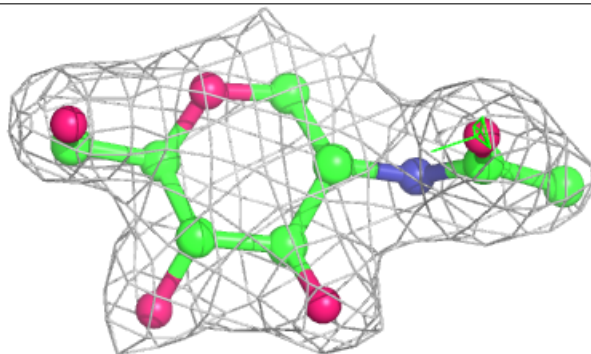


Electron density around NAG D 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

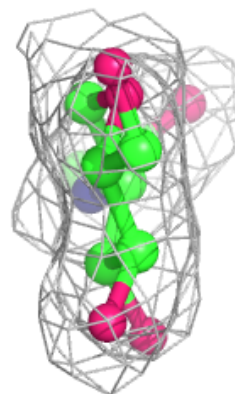
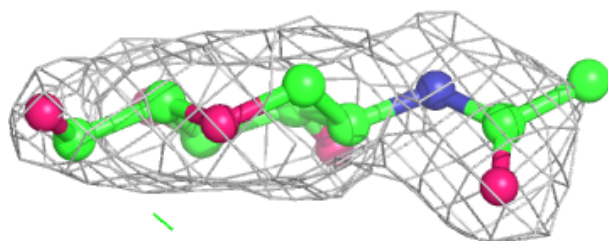
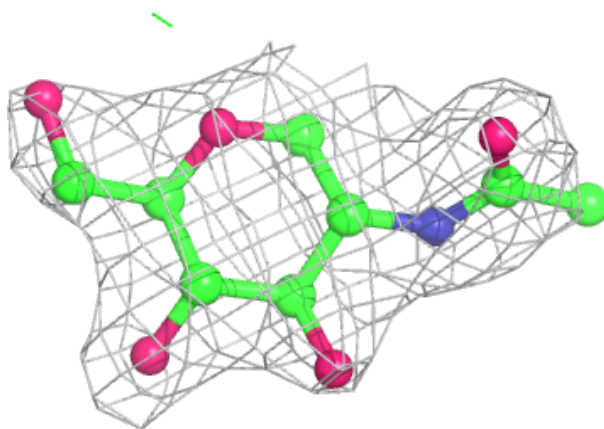
**Electron density around NAG A 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



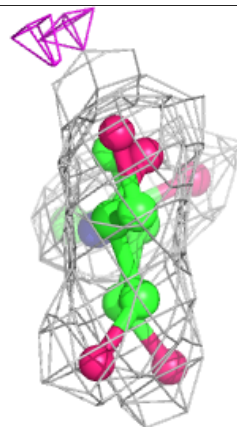
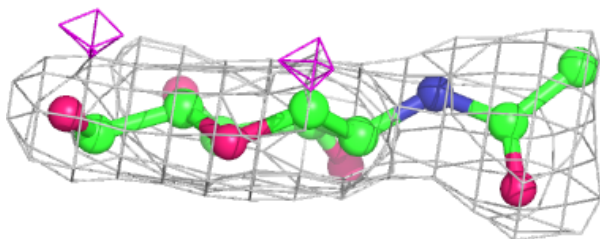
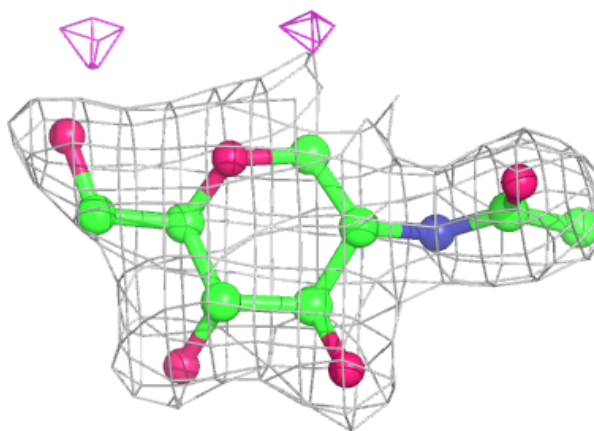
Electron density around NAG E 505:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

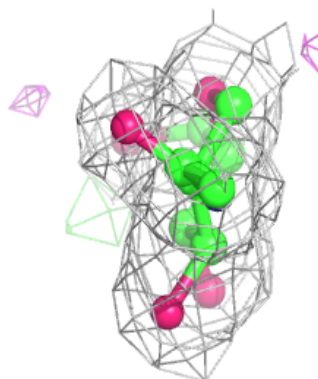
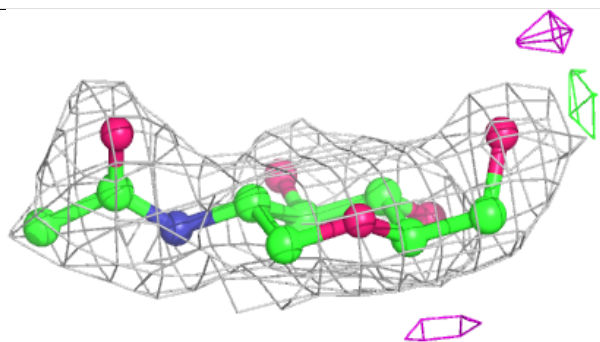
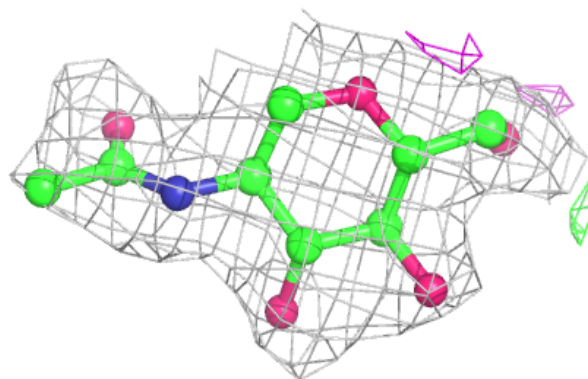


Electron density around NAG L 1003:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

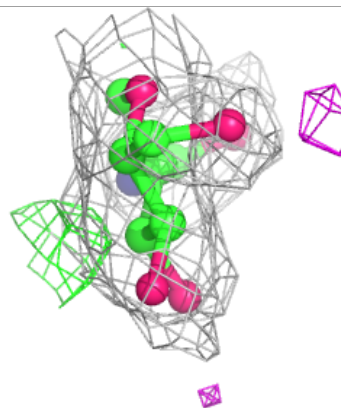
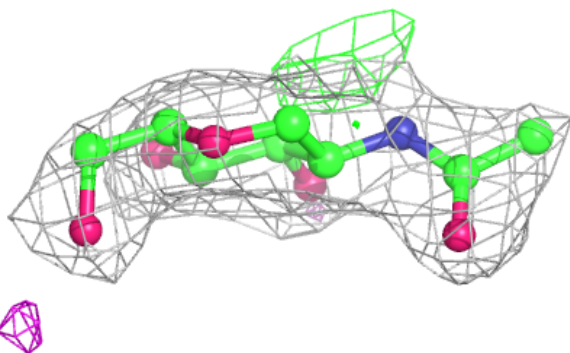
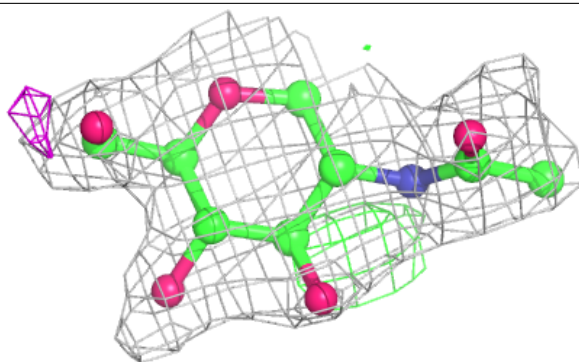
**Electron density around NAG A 504:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

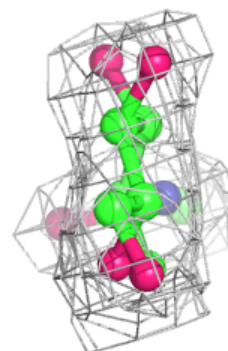
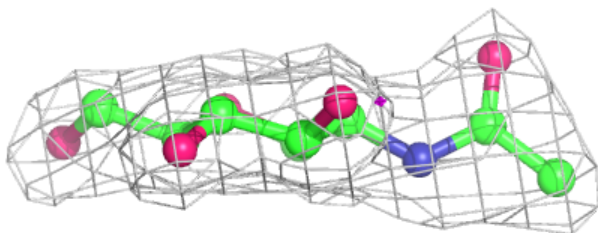
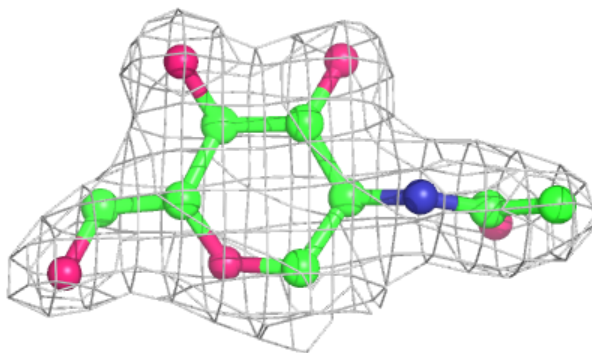


Electron density around NAG O 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

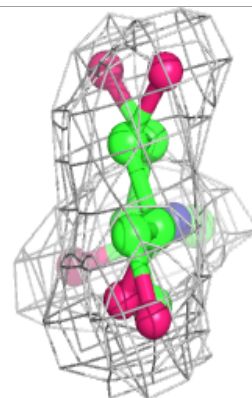
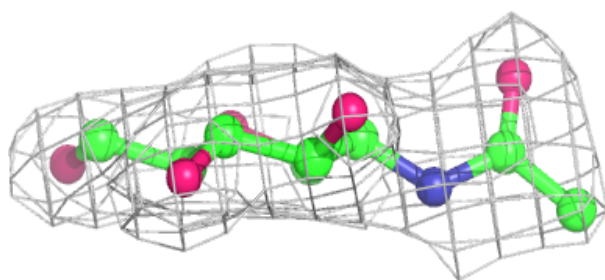
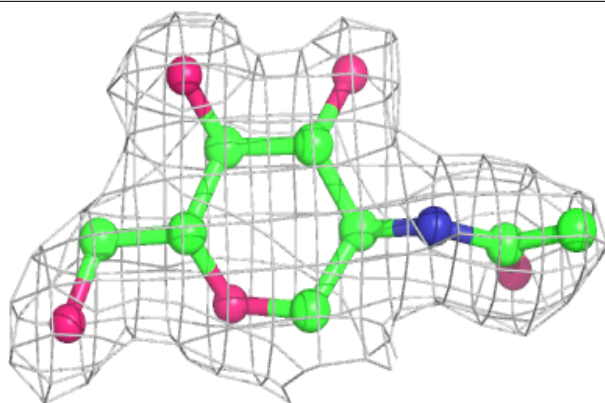
**Electron density around NAG H 1002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

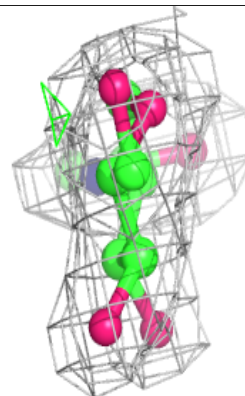
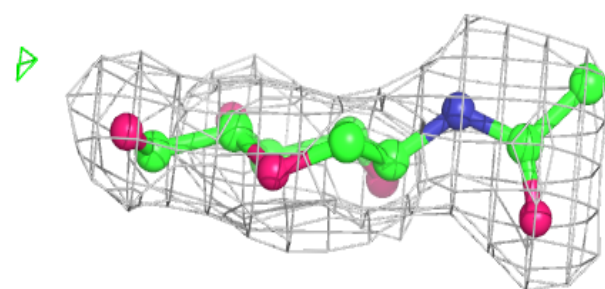
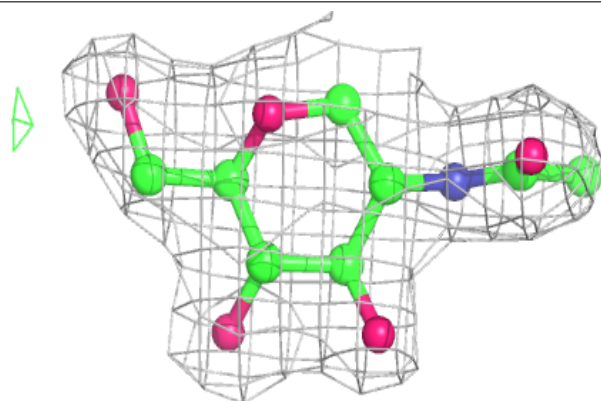


Electron density around NAG F 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

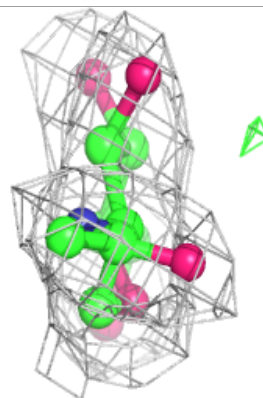
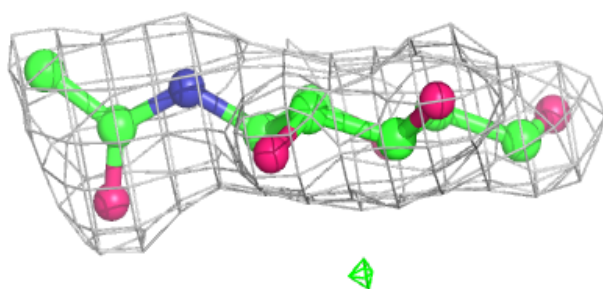
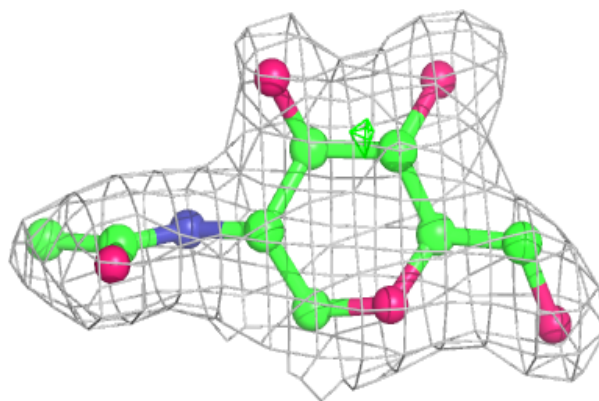
**Electron density around NAG N 1002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

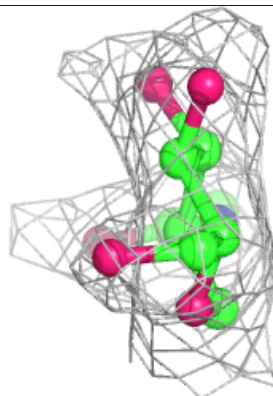
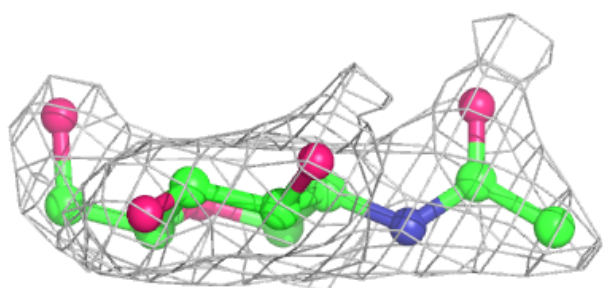
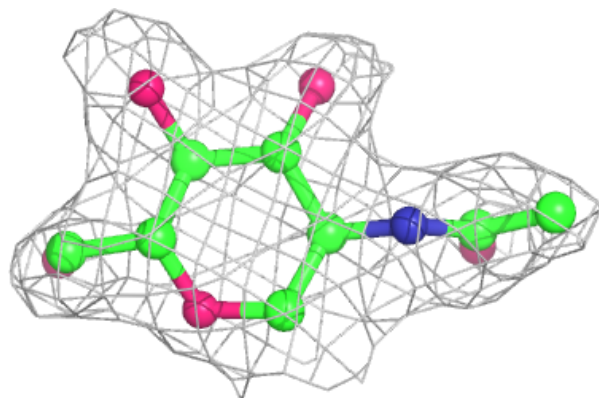


Electron density around NAG B 1003:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

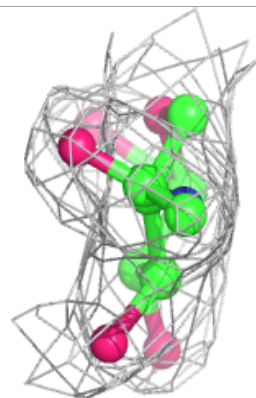
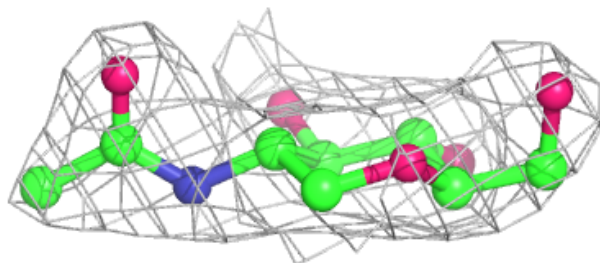
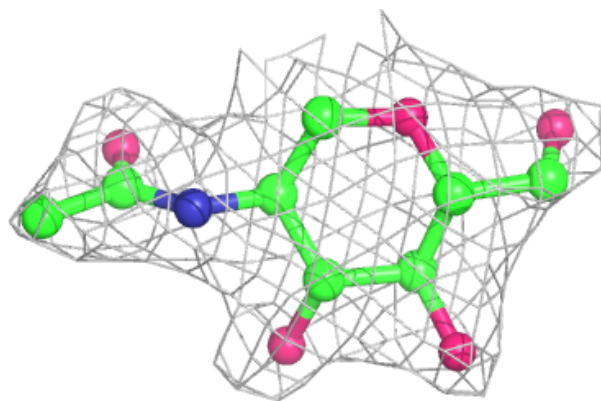
**Electron density around NAG C 502:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

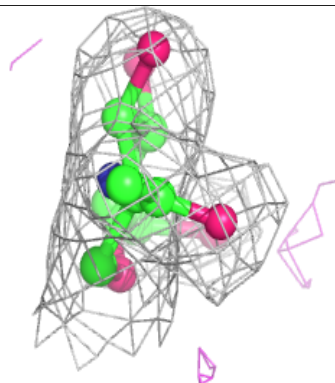
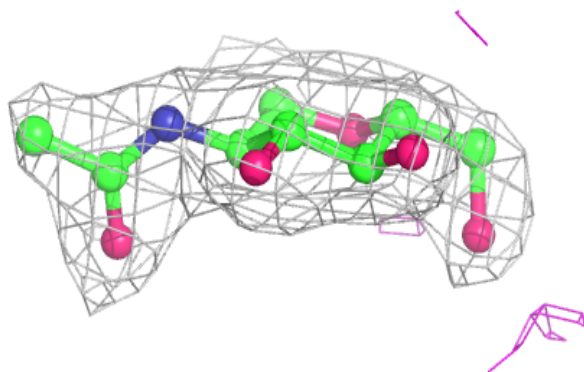
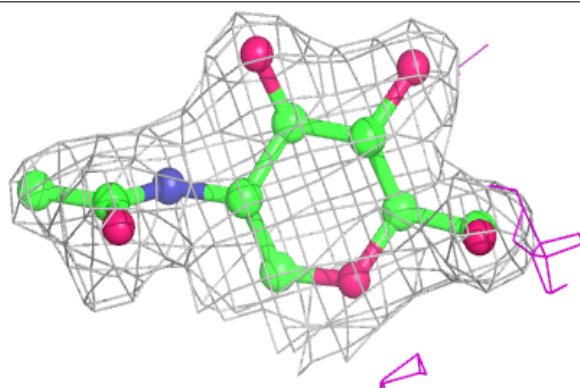


Electron density around NAG O 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

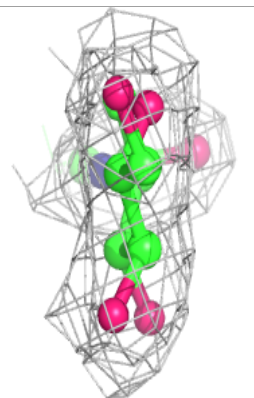
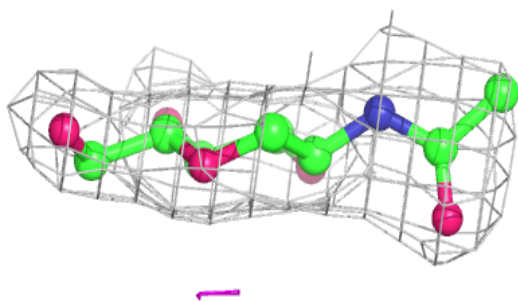
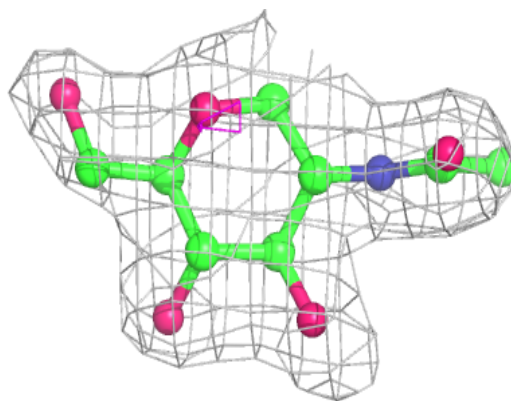
**Electron density around NAG I 504:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

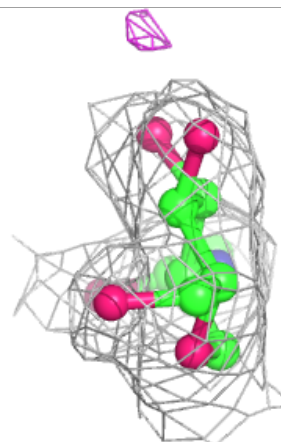
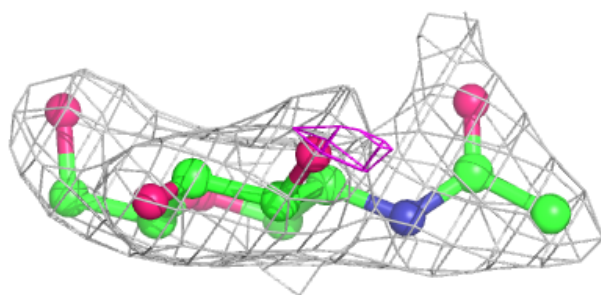
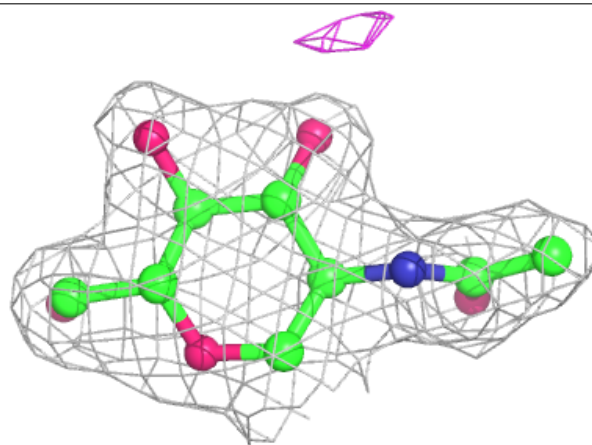


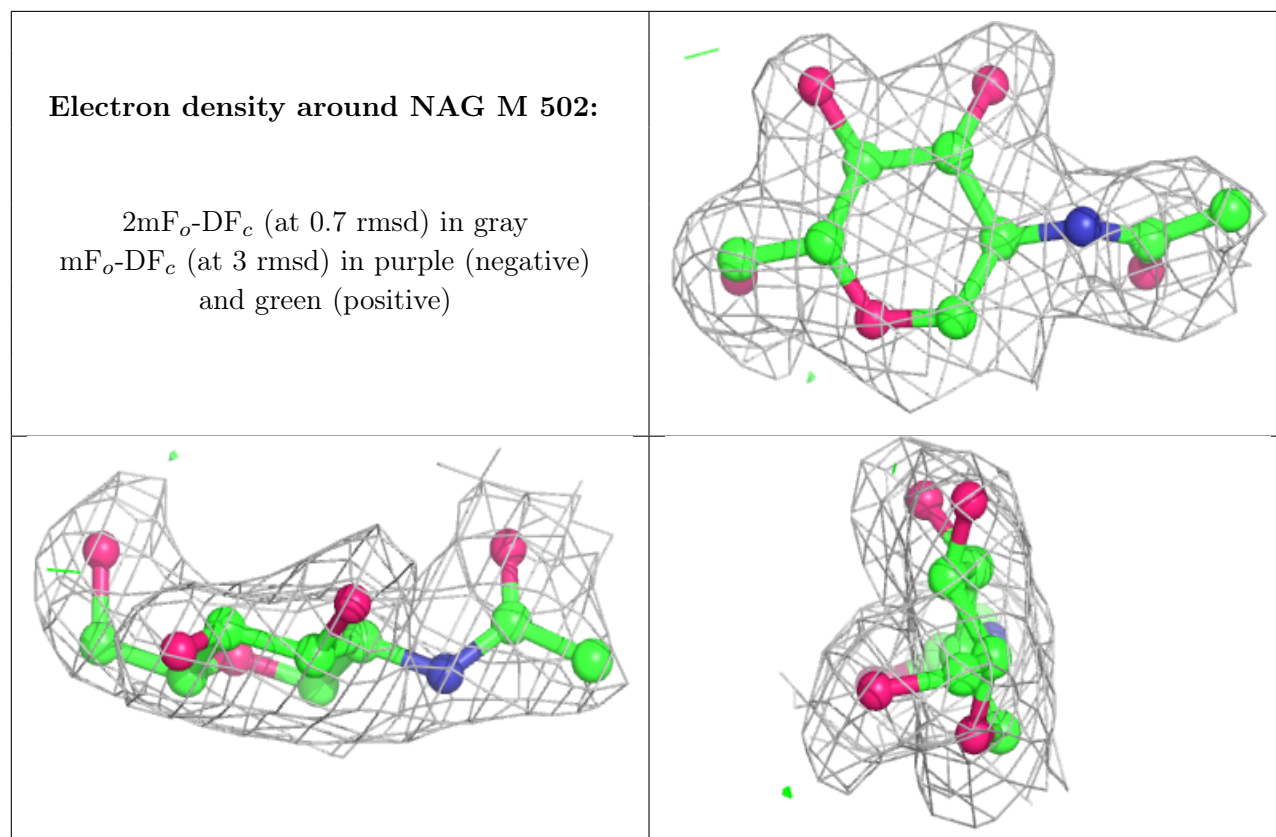
Electron density around NAG J 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAG I 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.