



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:16 PM UTC

PDB ID : 7XOI / pdb_00007xoi
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

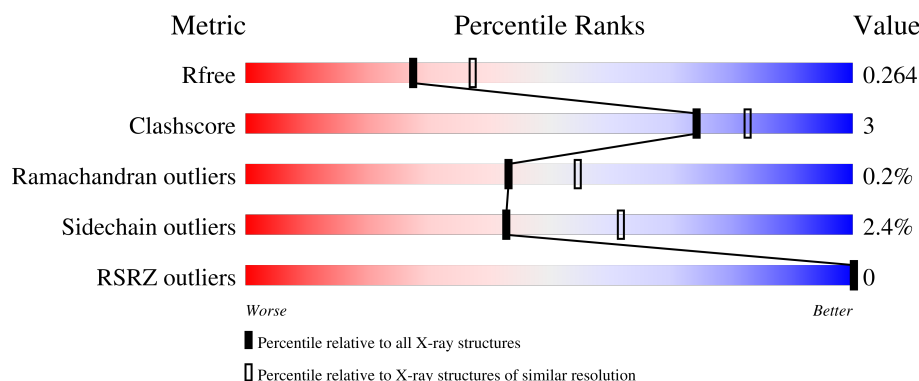
1 Overall quality at a glance

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.



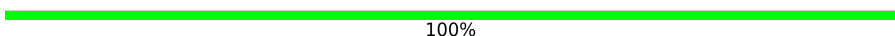
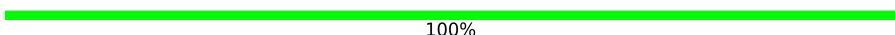
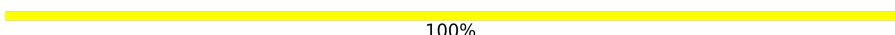
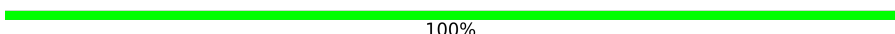
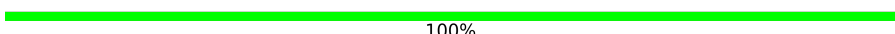
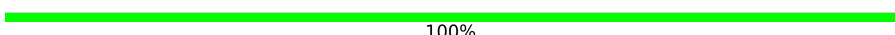
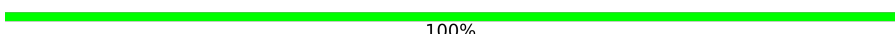
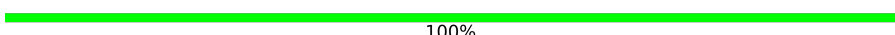
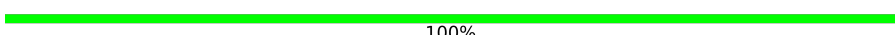
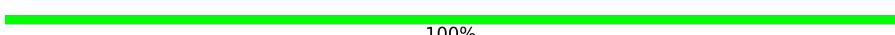
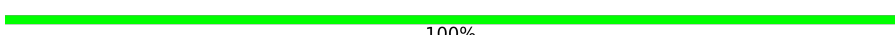
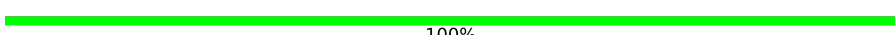
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	

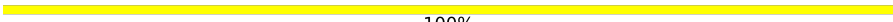
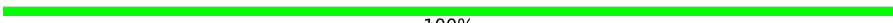
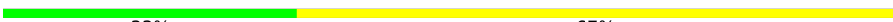
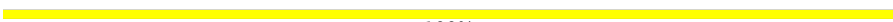
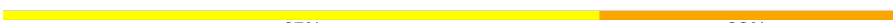
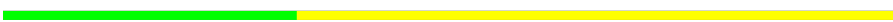
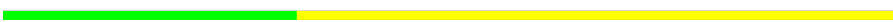
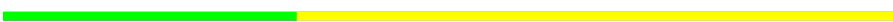
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Mol	Chain	Length	Quality of chain
1	K	548	 78%7%15%
1	M	548	 76%9%15%
1	O	548	 78%7%15%
2	B	445	 91%7%
2	D	445	 90%8%
2	F	445	 87%10%
2	H	445	 89%9%
2	J	445	 88%9%
2	L	445	 88%9%
2	N	445	 89%9%
2	P	445	 89%8%
3	Q	2	 100%
3	S	2	 100%
3	U	2	 100%
3	W	2	 100%
3	Y	2	 100%
3	a	2	 100%
3	c	2	 100%
3	e	2	 100%
3	g	2	 100%
3	i	2	 50%50%
3	k	2	 100%
3	m	2	 100%
3	o	2	 100%
3	q	2	 100%

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

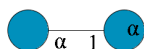
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	436	Total	C	N	O	S	0	0	0
			3397	2151	575	662	9			
2	D	436	Total	C	N	O	S	0	0	0
			3397	2151	575	662	9			
2	F	436	Total	C	N	O	S	0	0	0
			3397	2151	575	662	9			
2	H	436	Total	C	N	O	S	0	0	0
			3397	2151	575	662	9			
2	J	436	Total	C	N	O	S	0	0	0
			3397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



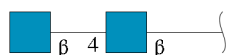
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	Q	2	Total	C	O	0	0	0
			23	12	11			
3	S	2	Total	C	O	0	0	0
			23	12	11			
3	U	2	Total	C	O	0	0	0
			23	12	11			
3	W	2	Total	C	O	0	0	0
			23	12	11			
3	Y	2	Total	C	O	0	0	0
			23	12	11			
3	a	2	Total	C	O	0	0	0
			23	12	11			
3	c	2	Total	C	O	0	0	0
			23	12	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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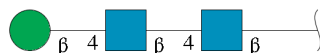
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	u	2	Total	C	O	0	0	0
			23	12	11			

- 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.



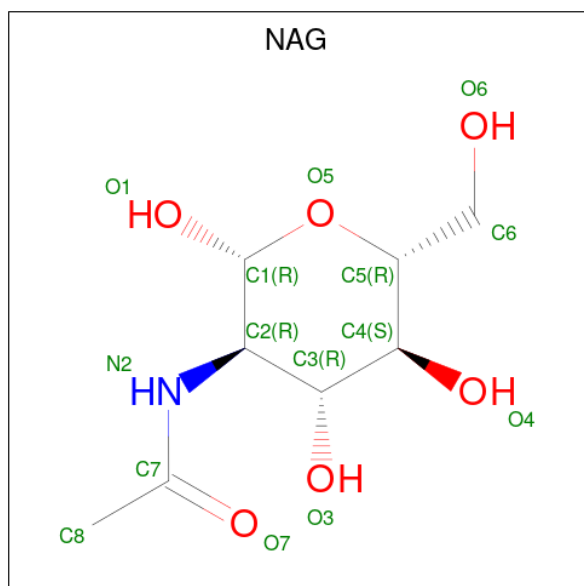
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	T	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	b	3	Total	C	N	O	0	0	0
			39	22	2	15			

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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 (CCD ID: 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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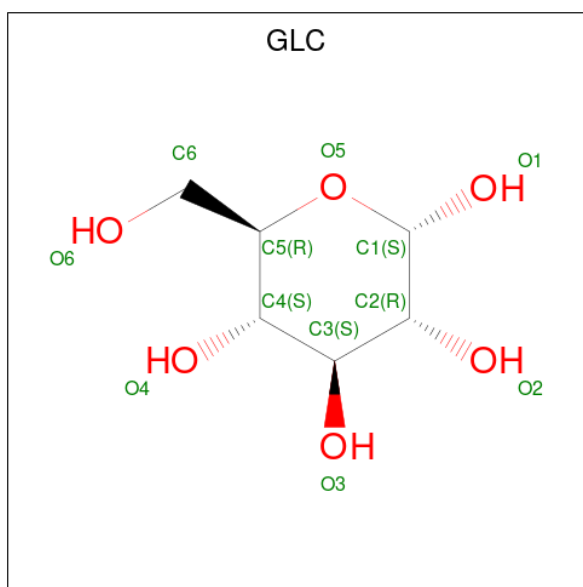
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	N	1	Total	C	N	O	0	0
			14	8	1	5		
6	N	1	Total	C	N	O	0	0
			14	8	1	5		
6	O	1	Total	C	N	O	0	0
			14	8	1	5		
6	O	1	Total	C	N	O	0	0
			14	8	1	5		
6	O	1	Total	C	N	O	0	0
			14	8	1	5		
6	O	1	Total	C	N	O	0	0
			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 (CCD ID: 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 (CCD ID: GLC) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is water.

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

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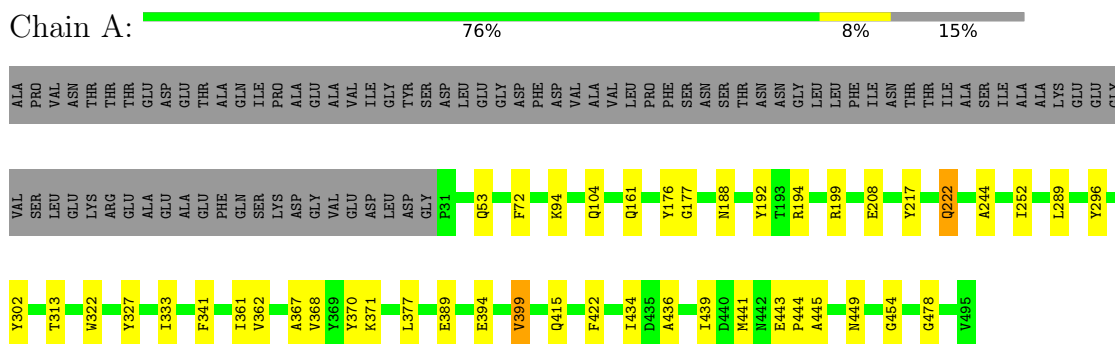
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	138	Total 138	O 138	0	0
9	F	128	Total 128	O 128	0	0
9	G	145	Total 145	O 145	0	0
9	H	114	Total 114	O 114	0	0
9	I	143	Total 143	O 143	0	0
9	J	105	Total 105	O 105	0	0
9	K	138	Total 138	O 138	0	0
9	L	101	Total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

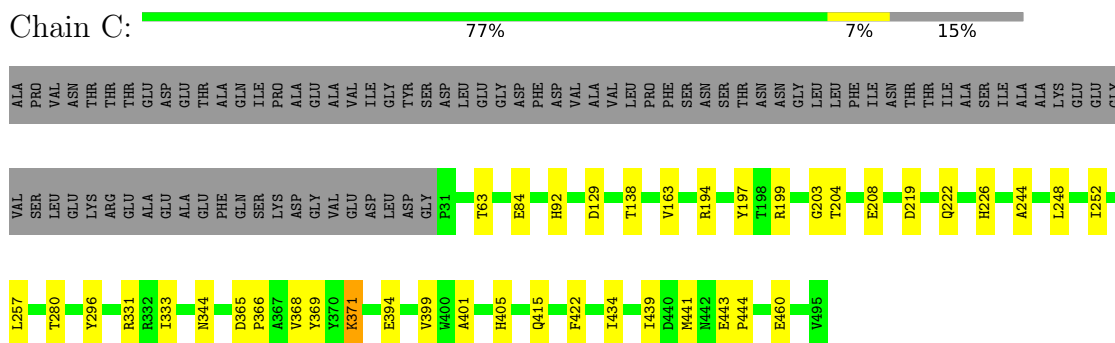
3 Residue-property plots

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.

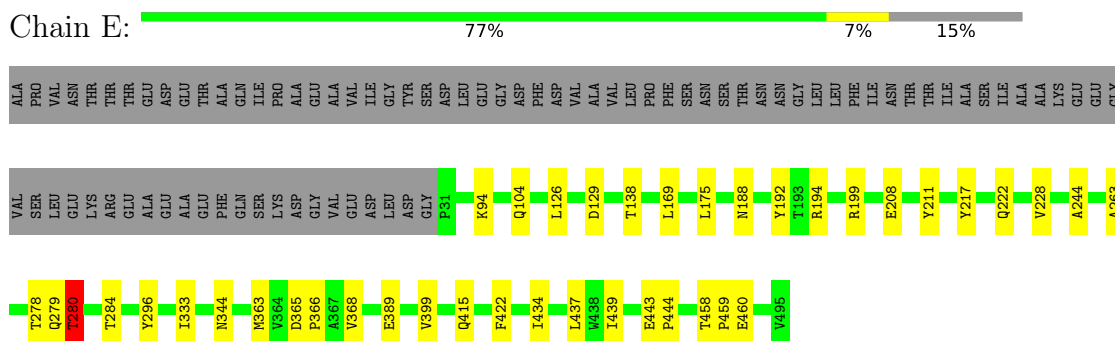
- Molecule 1: alpha-glucosidase N-terminal polypeptide



- Molecule 1: alpha-glucosidase N-terminal polypeptide

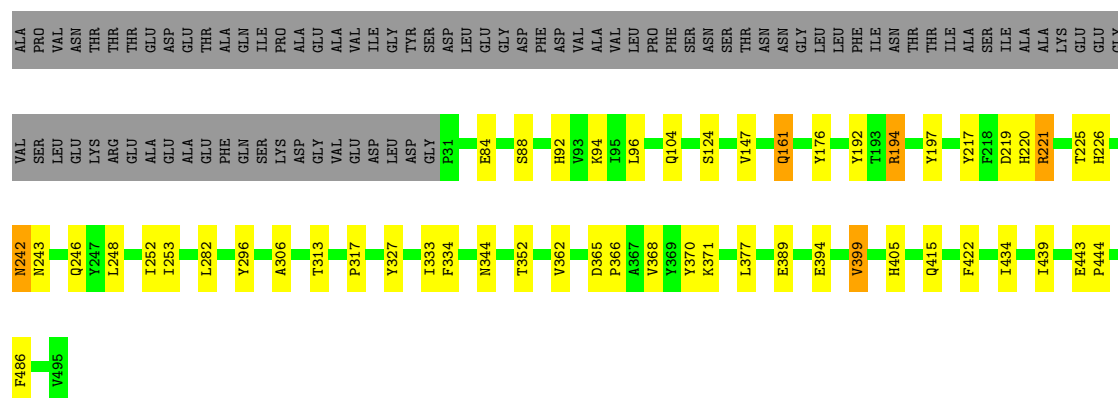


- Molecule 1: alpha-glucosidase N-terminal polypeptide



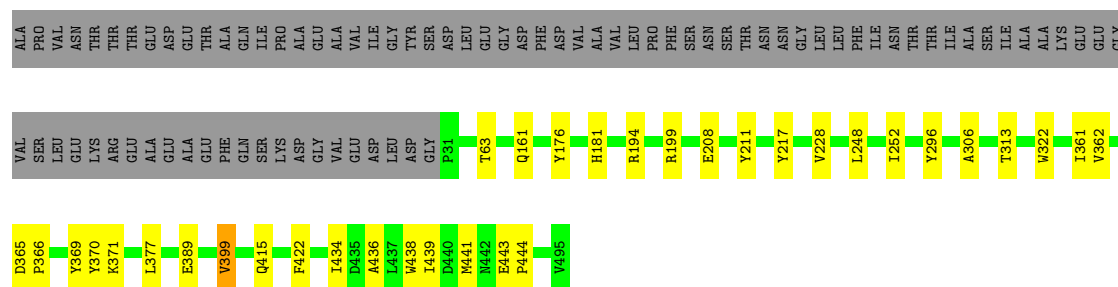
- Molecule 1: alpha-glucosidase N-terminal polypeptide

Chain G:  75% 9% 15%



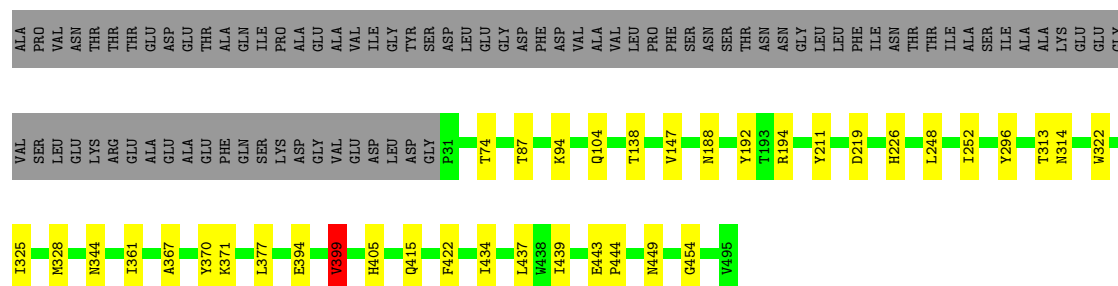
- Molecule 1: alpha-glucosidase N-terminal polypeptide

Chain I:  78% 6% 15%



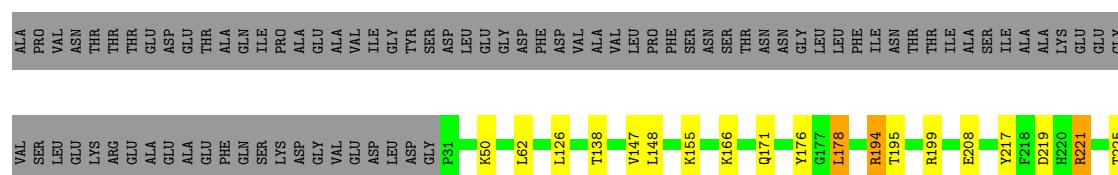
- Molecule 1: alpha-glucosidase N-terminal polypeptide

Chain K:  78% 7% 15%



- Molecule 1: alpha-glucosidase N-terminal polypeptide

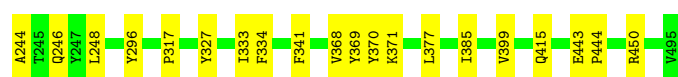
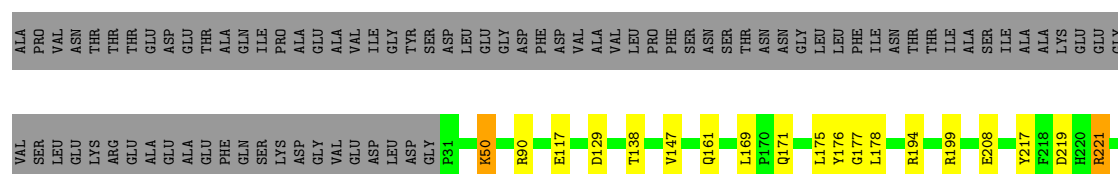
Chain M:  76% 9% 15%





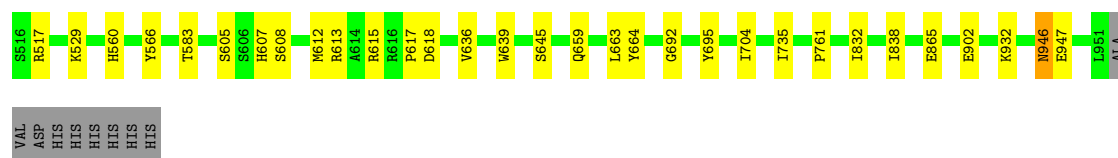
- Molecule 1: alpha-glucosidase N-terminal polypeptide

Chain O: 78% 7% 15%



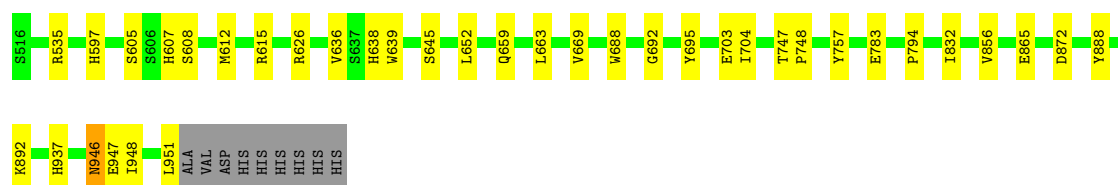
- Molecule 2: alpha-glucosidase C-terminal polypeptide

Chain B: 91% 7% .



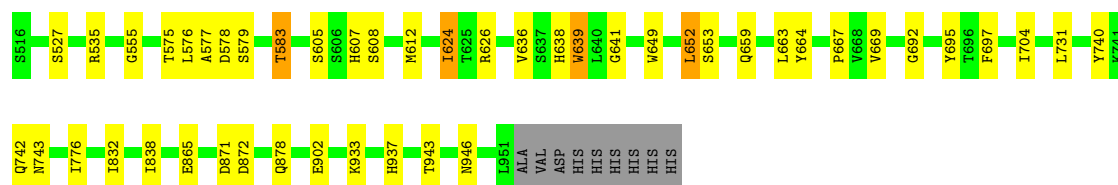
- Molecule 2: alpha-glucosidase C-terminal polypeptide

Chain D: 90% 8% .



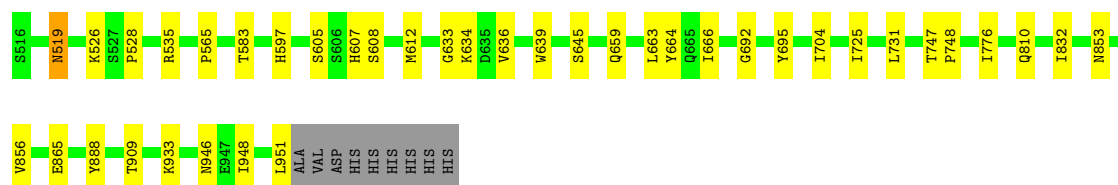
- Molecule 2: alpha-glucosidase C-terminal polypeptide

Chain F: 87% 10% ..



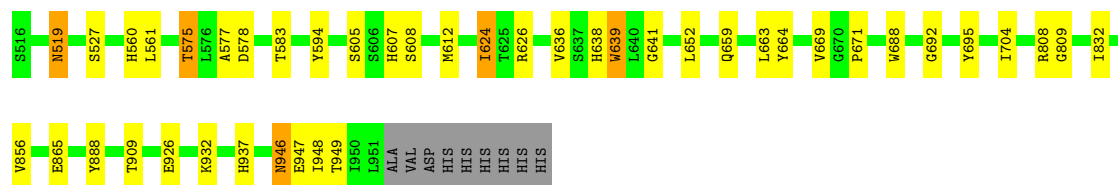
- Molecule 2: alpha-glucosidase C-terminal polypeptide

Chain H:  89% 9% .



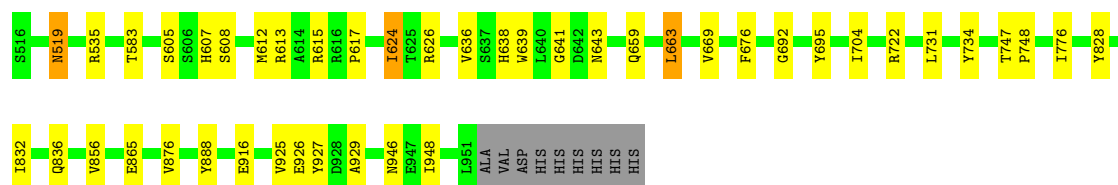
- Molecule 2: alpha-glucosidase C-terminal polypeptide

Chain J:  88% 9% ..



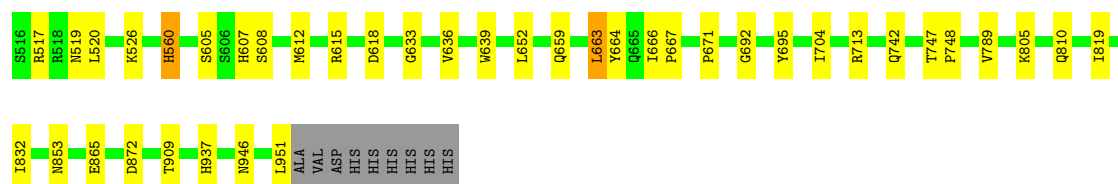
- Molecule 2: alpha-glucosidase C-terminal polypeptide

Chain L:  88% 9% ..



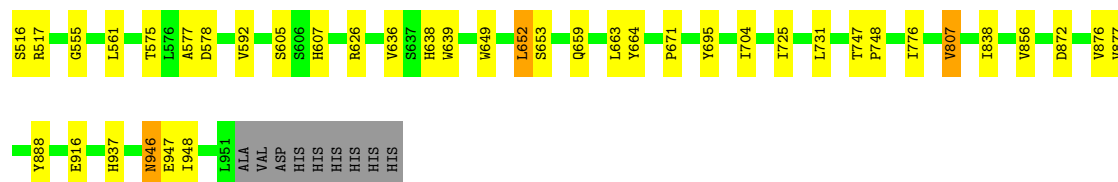
- Molecule 2: alpha-glucosidase C-terminal polypeptide

Chain N:  89% 9% .



- Molecule 2: alpha-glucosidase C-terminal polypeptide

Chain P:  89% 8% ..



- 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%

MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2

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

Chain V:  50% 50%

MAG1
MAG2

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

Chain Z:  100%

MAG1
MAG2

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

Chain d:  50% 50%

MAG1
MAG2

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

Chain h:  50% 50%

MAG1
MAG2

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

Chain l:  50% 50%

MAG1
MAG2

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

Chain p:  50% 50%

MAG1
MAG2

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

Chain t:  100%

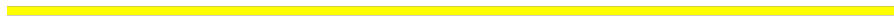
MAG1
MAG2

- 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:  33% 67%

MAG1
MAG2
EMA3

- 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%

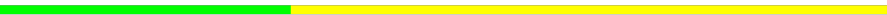
MAG1
MAG2
EMA3

- 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:  67% 33%

MAG1
MAG2
EMA3

- 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%

MAG1
MAG2
EMA3

- 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%



- 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:  33% 67%



- 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%



- 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%



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 49.14 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.14-2.30) 94.4 (49.14-2.30)	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 (4.73%)	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 , 5.2	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	0.95	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.96	0/3875	1.29	0/5306
1	C	0.97	0/3875	1.30	1/5306 (0.0%)
1	E	0.96	0/3875	1.30	1/5306 (0.0%)
1	G	0.97	0/3875	1.31	0/5306
1	I	0.97	0/3875	1.30	0/5306
1	K	0.96	0/3875	1.28	0/5306
1	M	0.96	0/3875	1.29	0/5306
1	O	0.97	0/3875	1.30	0/5306
2	B	0.99	0/3487	1.33	2/4755 (0.0%)
2	D	1.00	0/3487	1.35	0/4755
2	F	0.99	0/3487	1.35	1/4755 (0.0%)
2	H	1.00	0/3487	1.33	0/4755
2	J	1.00	0/3487	1.33	0/4755
2	L	1.00	0/3487	1.34	0/4755
2	N	1.00	0/3487	1.34	0/4755
2	P	1.00	0/3487	1.34	1/4755 (0.0%)
All	All	0.98	0/58896	1.32	6/80488 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	555	GLY	CA-C-O	-6.36	118.09	122.22
2	F	555	GLY	CA-C-O	-6.01	118.31	122.22
1	E	280	THR	CB-CA-C	5.57	118.17	109.42
2	B	529	LYS	CA-C-N	5.52	125.34	120.10
2	B	529	LYS	C-N-CA	5.52	125.34	120.10
1	C	280	THR	CB-CA-C	5.33	117.94	109.52

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	30	0
1	C	3747	0	3459	24	0
1	E	3747	0	3459	25	0
1	G	3747	0	3459	34	0
1	I	3747	0	3459	25	0
1	K	3747	0	3461	24	0
1	M	3747	0	3459	30	0
1	O	3747	0	3459	22	0
2	B	3397	0	3217	21	0
2	D	3397	0	3218	27	0
2	F	3397	0	3217	34	0
2	H	3397	0	3216	23	0
2	J	3397	0	3216	31	0
2	L	3397	0	3216	30	0
2	N	3397	0	3217	26	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Z	28	0	25	0	0
4	d	28	0	25	1	0
4	h	28	0	25	1	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	2	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	350	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.

All (350) 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
2:N:605:SER:HB3	2:N:636:VAL:HG11	1.65	0.78
2:F:652:LEU:C	2:F:652:LEU:HD23	2.10	0.77
2:P:652:LEU:C	2:P:652:LEU:HD23	2.10	0.77
1:G:443:GLU:N	1:G:444:PRO:HA	2.02	0.75
1:C:443:GLU:N	1:C:444:PRO:HA	1.99	0.74
1:M:415:GLN:HE22	2:N:607:HIS:HA	1.52	0.74
1:K:443:GLU:N	1:K:444:PRO:HA	2.02	0.74
2:L:605:SER:HB3	2:L:636:VAL:HG11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:443:GLU:N	1:O:444:PRO:HA	2.02	0.73
1:M:443:GLU:N	1:M:444:PRO:HA	2.04	0.72
1:A:443:GLU:N	1:A:444:PRO:HA	2.04	0.72
2:J:605:SER:HB3	2:J:636:VAL:HG11	1.71	0.71
2:F:605:SER:HB3	2:F:636:VAL:HG11	1.72	0.71
1:E:443:GLU:N	1:E:444:PRO:HA	2.05	0.71
1:I:443:GLU:N	1:I:444:PRO:HA	2.06	0.71
2:D:612:MET:HE2	2:D:615:ARG:HD3	1.73	0.70
1:C:422:PHE:CD2	2:D:612:MET:HE3	2.26	0.70
2:B:605:SER:HB3	2:B:636:VAL:HG11	1.74	0.69
1:G:434:ILE:HD11	2:H:612:MET:HE1	1.75	0.68
1:C:422:PHE:HD2	2:D:612:MET:HE3	1.60	0.66
1:G:415:GLN:HE22	2:H:607:HIS:HA	1.60	0.65
2:J:624:ILE:HD13	2:J:624:ILE:O	1.97	0.64
2:L:612:MET:HE2	2:L:615:ARG:HD3	1.80	0.64
1:E:458:THR:HG22	1:E:459:PRO:HD2	1.81	0.63
2:J:832:ILE:HA	2:J:865:GLU:O	1.97	0.63
2:N:517:ARG:NH2	2:N:618:ASP:OD1	2.32	0.62
1:C:296:TYR:O	2:D:704:ILE:HA	1.98	0.62
1:A:415:GLN:HE22	2:B:607:HIS:HA	1.64	0.62
2:J:575:THR:HB	2:J:578:ASP:OD1	2.00	0.61
2:J:937:HIS:HB3	1:M:313:THR:O	2.00	0.61
2:F:731:LEU:HD13	2:F:776:ILE:HD13	1.82	0.61
2:N:659:GLN:O	2:N:663:LEU:HB2	2.01	0.60
2:P:659:GLN:O	2:P:663:LEU:HB2	2.03	0.59
2:D:937:HIS:HB3	1:G:313:THR:O	2.03	0.58
1:G:161:GLN:HG2	2:H:565:PRO:HD2	1.85	0.58
1:C:199:ARG:NH2	1:C:208:GLU:OE2	2.36	0.58
1:K:296:TYR:O	2:L:704:ILE:HA	2.04	0.58
1:E:434:ILE:HD11	2:F:612:MET:HE1	1.86	0.58
1:M:422:PHE:CD2	2:N:612:MET:HE3	2.39	0.58
2:H:659:GLN:O	2:H:663:LEU:HB2	2.05	0.56
2:N:692:GLY:HA2	2:N:695:TYR:CD2	2.40	0.56
1:E:280:THR:HG21	5:b:1:NAG:HN2	1.71	0.56
2:B:659:GLN:O	2:B:663:LEU:HB2	2.05	0.56
2:D:659:GLN:O	2:D:663:LEU:HB2	2.06	0.56
2:F:624:ILE:HG13	2:F:624:ILE:O	2.04	0.56
1:E:415:GLN:HE22	2:F:607:HIS:HA	1.70	0.55
2:F:832:ILE:HA	2:F:865:GLU:O	2.07	0.55
2:J:659:GLN:O	2:J:663:LEU:HB2	2.06	0.55
2:N:832:ILE:HA	2:N:865:GLU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:ILE:HD11	2:F:608:SER:CB	2.37	0.55
2:P:649:TRP:HA	2:P:652:LEU:HD22	1.88	0.55
1:A:370:TYR:HA	1:A:377:LEU:HD22	1.89	0.55
2:H:692:GLY:HA2	2:H:695:TYR:CD2	2.41	0.55
1:O:147:VAL:O	1:O:221:ARG:NH1	2.39	0.54
1:O:176:TYR:O	1:O:217:TYR:HA	2.07	0.54
1:A:176:TYR:O	1:A:217:TYR:HA	2.07	0.54
1:M:333:ILE:HD11	1:M:368:VAL:HG22	1.89	0.54
2:L:731:LEU:HD13	2:L:776:ILE:HD13	1.90	0.54
1:E:296:TYR:O	2:F:704:ILE:HA	2.06	0.54
1:K:370:TYR:HA	1:K:377:LEU:HD22	1.90	0.54
2:D:692:GLY:HA2	2:D:695:TYR:CD2	2.43	0.53
2:P:652:LEU:HD23	2:P:653:SER:N	2.22	0.53
1:I:322:TRP:CH2	2:J:624:ILE:HD12	2.43	0.53
2:L:659:GLN:O	2:L:663:LEU:HB2	2.08	0.53
1:E:333:ILE:HD11	1:E:368:VAL:HG22	1.91	0.53
1:M:422:PHE:HD2	2:N:612:MET:CE	2.21	0.53
2:P:659:GLN:HB3	2:P:664:TYR:CE2	2.43	0.53
2:L:692:GLY:HA2	2:L:695:TYR:CD2	2.44	0.53
2:F:692:GLY:HA2	2:F:695:TYR:CD2	2.43	0.53
1:K:192:TYR:CE2	1:K:194:ARG:HG2	2.44	0.53
1:A:296:TYR:O	2:B:704:ILE:HA	2.09	0.52
2:F:638:HIS:CE1	2:F:639:TRP:O	2.62	0.52
1:I:322:TRP:HH2	2:J:624:ILE:HD12	1.72	0.52
1:O:370:TYR:HA	1:O:377:LEU:HD22	1.91	0.52
2:H:731:LEU:HD13	2:H:776:ILE:HD13	1.90	0.52
2:F:659:GLN:O	2:F:663:LEU:HB2	2.10	0.52
2:D:946:ASN:HD22	2:D:947:GLU:H	1.56	0.52
1:G:147:VAL:O	1:G:221:ARG:NH1	2.43	0.52
1:I:362:VAL:HG22	1:I:434:ILE:HG21	1.91	0.52
1:A:422:PHE:CE2	2:B:612:MET:HE3	2.46	0.51
1:I:415:GLN:HE22	2:J:607:HIS:HA	1.75	0.51
1:O:333:ILE:HD11	1:O:368:VAL:HG22	1.91	0.51
1:E:211:TYR:CE2	2:F:641:GLY:HA3	2.46	0.51
2:B:946:ASN:HD22	2:B:947:GLU:H	1.59	0.51
1:G:296:TYR:O	2:H:704:ILE:HA	2.11	0.51
1:M:199:ARG:NH2	1:M:208:GLU:OE2	2.44	0.51
1:G:192:TYR:CE2	1:G:194:ARG:HG2	2.45	0.51
1:K:415:GLN:HE22	2:L:607:HIS:HA	1.76	0.50
2:F:649:TRP:HA	2:F:652:LEU:HD22	1.93	0.50
1:E:439:ILE:HD11	2:F:608:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:370:TYR:HA	1:G:377:LEU:HD22	1.93	0.50
1:G:333:ILE:HD12	1:G:334:PHE:CE2	2.46	0.50
1:C:434:ILE:HD11	2:D:612:MET:HE1	1.93	0.49
1:A:439:ILE:HD11	2:B:608:SER:CB	2.42	0.49
1:O:129:ASP:HB2	1:O:138:THR:CG2	2.41	0.49
1:O:317:PRO:HB2	2:P:725:ILE:HG21	1.94	0.49
1:M:166:LYS:HD2	1:M:247:TYR:CD1	2.47	0.49
1:K:439:ILE:HD11	2:L:608:SER:CB	2.43	0.49
1:G:248:LEU:C	1:G:248:LEU:HD23	2.37	0.49
1:M:439:ILE:HD11	2:N:608:SER:CB	2.43	0.49
1:E:94:LYS:NZ	1:E:104:GLN:HE22	2.11	0.48
1:I:199:ARG:NH2	1:I:208:GLU:OE2	2.46	0.48
5:T:2:NAG:H4	5:T:3:BMA:O2	2.12	0.48
2:N:692:GLY:HA2	2:N:695:TYR:CE2	2.49	0.48
2:P:856:VAL:HG11	2:P:888:TYR:CG	2.48	0.48
2:D:832:ILE:HA	2:D:865:GLU:O	2.13	0.48
2:H:692:GLY:HA2	2:H:695:TYR:CE2	2.49	0.48
1:M:296:TYR:O	2:N:704:ILE:HA	2.13	0.48
1:A:313:THR:O	2:F:937:HIS:HB3	2.14	0.48
2:D:626:ARG:O	2:D:638:HIS:CE1	2.66	0.48
1:E:280:THR:CG2	5:b:1:NAG:HN2	2.26	0.48
1:M:225:THR:HG22	1:M:270:VAL:HG21	1.95	0.48
1:M:230:LEU:HD23	1:M:236:MET:HE1	1.95	0.48
1:M:365:ASP:HB2	1:M:366:PRO:HD2	1.96	0.48
2:D:872:ASP:C	2:D:872:ASP:OD1	2.57	0.48
1:K:422:PHE:CD2	2:L:612:MET:HE3	2.49	0.48
1:A:199:ARG:NH2	1:A:208:GLU:OE2	2.46	0.48
2:B:612:MET:HE2	2:B:615:ARG:HD3	1.96	0.47
2:B:832:ILE:HA	2:B:865:GLU:O	2.14	0.47
1:E:278:THR:O	1:E:279:GLN:HB2	2.14	0.47
1:M:422:PHE:CE2	2:N:612:MET:HE3	2.50	0.47
2:P:575:THR:HB	2:P:578:ASP:OD2	2.13	0.47
1:C:84:GLU:HB2	1:C:92:HIS:HB3	1.96	0.47
1:K:211:TYR:CE2	2:L:641:GLY:HA3	2.50	0.47
1:O:178:LEU:HG	1:O:217:TYR:HB3	1.97	0.47
1:O:369:TYR:CZ	1:O:371:LYS:HB2	2.50	0.47
2:J:692:GLY:HA2	2:J:695:TYR:CE2	2.50	0.47
2:L:828:TYR:OH	2:L:836:GLN:NE2	2.44	0.47
1:I:217:TYR:CE2	1:I:228:VAL:HB	2.50	0.47
1:O:50:LYS:HE2	1:O:50:LYS:HA	1.97	0.47
1:E:437:LEU:CD2	2:F:608:SER:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:652:LEU:C	2:F:652:LEU:CD2	2.82	0.47
1:G:327:TYR:CE2	1:G:362:VAL:HB	2.50	0.47
1:C:439:ILE:HD11	2:D:608:SER:HB2	1.96	0.47
1:K:313:THR:O	2:P:937:HIS:HB3	2.15	0.47
1:K:322:TRP:HA	1:K:361:ILE:O	2.15	0.47
1:O:248:LEU:HD23	1:O:248:LEU:C	2.40	0.47
1:O:296:TYR:O	2:P:704:ILE:HA	2.15	0.47
1:G:282:LEU:HB3	2:H:634:LYS:O	2.15	0.47
2:J:856:VAL:HG11	2:J:888:TYR:CG	2.49	0.46
2:P:671:PRO:HD2	2:P:695:TYR:CD2	2.50	0.46
2:D:652:LEU:HD12	2:D:652:LEU:C	2.40	0.46
2:D:703:GLU:HG2	2:D:704:ILE:N	2.29	0.46
1:G:306:ALA:HB3	4:d:1:NAG:H82	1.95	0.46
1:A:94:LYS:NZ	1:A:104:GLN:HE22	2.12	0.46
1:A:222:GLN:HE21	2:B:761:PRO:HG3	1.81	0.46
2:N:872:ASP:C	2:N:872:ASP:OD1	2.58	0.46
1:A:422:PHE:CD2	2:B:612:MET:HE3	2.51	0.46
2:D:856:VAL:HG11	2:D:888:TYR:CG	2.51	0.46
2:N:560:HIS:N	2:N:560:HIS:CD2	2.84	0.46
2:P:671:PRO:HD2	2:P:695:TYR:CE2	2.50	0.46
1:C:163:VAL:HG12	1:C:257:LEU:HD21	1.97	0.46
2:F:652:LEU:HD23	2:F:653:SER:N	2.31	0.46
2:L:832:ILE:HA	2:L:865:GLU:O	2.16	0.46
1:M:422:PHE:CD2	2:N:612:MET:CE	2.98	0.46
1:A:439:ILE:HD11	2:B:608:SER:HB2	1.97	0.46
1:C:331:ARG:O	1:C:401:ALA:HB2	2.16	0.46
1:K:325:ILE:HG13	1:K:328:MET:SD	2.56	0.46
2:L:613:ARG:O	2:L:617:PRO:HA	2.14	0.46
1:O:443:GLU:N	1:O:444:PRO:CA	2.78	0.46
2:F:731:LEU:CD1	2:F:776:ILE:HD13	2.45	0.46
1:I:422:PHE:CE2	2:J:612:MET:HE3	2.51	0.46
2:J:659:GLN:HB3	2:J:664:TYR:CE2	2.51	0.46
2:N:853:ASN:OD1	2:N:909:THR:HG23	2.16	0.46
2:F:626:ARG:O	2:F:638:HIS:CE1	2.69	0.46
1:K:314:ASN:O	2:L:722:ARG:NH2	2.45	0.46
2:J:652:LEU:C	2:J:652:LEU:HD12	2.41	0.45
2:P:731:LEU:HD13	2:P:776:ILE:HD13	1.97	0.45
1:A:361:ILE:HG12	1:A:436:ALA:HB3	1.98	0.45
1:A:72:PHE:CG	2:B:566:TYR:HB2	2.51	0.45
1:I:369:TYR:CZ	1:I:371:LYS:HB2	2.52	0.45
1:I:370:TYR:HA	1:I:377:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:638:HIS:CE1	2:J:639:TRP:O	2.69	0.45
2:F:624:ILE:HD13	2:F:697:PHE:CZ	2.52	0.45
1:I:439:ILE:HD11	2:J:608:SER:HB2	1.98	0.45
1:M:138:THR:HG23	1:M:147:VAL:HG13	1.98	0.45
1:E:422:PHE:CE2	2:F:612:MET:HE3	2.52	0.45
2:J:561:LEU:HA	2:J:594:TYR:CD2	2.52	0.45
2:L:927:TYR:CE2	2:L:929:ALA:HA	2.52	0.45
1:E:188:ASN:HB2	1:E:192:TYR:CD1	2.52	0.45
1:G:439:ILE:HD11	2:H:608:SER:CB	2.47	0.45
1:K:437:LEU:CD2	2:L:608:SER:HB3	2.46	0.45
1:M:148:LEU:HB3	1:M:226:HIS:CE1	2.52	0.45
2:P:517:ARG:HD3	2:P:877:VAL:HB	1.98	0.45
1:A:441:MET:HB3	1:A:445:ALA:HB3	1.99	0.45
2:F:692:GLY:HA2	2:F:695:TYR:CE2	2.52	0.45
1:G:443:GLU:N	1:G:444:PRO:CA	2.78	0.45
1:K:248:LEU:C	1:K:248:LEU:HD23	2.42	0.45
1:M:394:GLU:HB2	1:M:405:HIS:CE1	2.52	0.45
1:A:322:TRP:HA	1:A:361:ILE:O	2.16	0.45
2:B:659:GLN:HB3	2:B:664:TYR:CE2	2.52	0.45
1:E:129:ASP:HB2	1:E:138:THR:CG2	2.47	0.45
1:E:199:ARG:NH2	1:E:208:GLU:OE2	2.50	0.45
2:F:575:THR:HB	2:F:578:ASP:OD2	2.16	0.45
2:P:626:ARG:O	2:P:638:HIS:CE1	2.70	0.45
1:A:333:ILE:HD11	1:A:368:VAL:HG22	1.99	0.45
1:E:126:LEU:HG	1:E:263:ALA:HB2	1.99	0.45
1:G:333:ILE:HD11	1:G:368:VAL:HG22	1.98	0.44
2:H:659:GLN:HB3	2:H:664:TYR:CE2	2.52	0.44
2:N:659:GLN:HB3	2:N:664:TYR:CE2	2.51	0.44
1:A:161:GLN:NE2	2:B:560:HIS:O	2.50	0.44
1:M:176:TYR:O	1:M:217:TYR:HA	2.17	0.44
1:A:362:VAL:HG22	1:A:434:ILE:HG21	1.99	0.44
1:C:415:GLN:HE22	2:D:607:HIS:HA	1.82	0.44
2:L:626:ARG:O	2:L:638:HIS:CE1	2.70	0.44
1:G:439:ILE:HD11	2:H:608:SER:HB2	1.99	0.44
1:C:129:ASP:HB2	1:C:138:THR:CG2	2.48	0.44
2:F:659:GLN:HB3	2:F:664:TYR:CE2	2.52	0.44
2:J:692:GLY:HA2	2:J:695:TYR:CD2	2.52	0.44
1:K:94:LYS:NZ	1:K:104:GLN:HE22	2.15	0.44
1:E:188:ASN:HB2	1:E:192:TYR:CG	2.52	0.44
1:C:248:LEU:C	1:C:248:LEU:HD23	2.42	0.44
1:C:333:ILE:HD11	1:C:368:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:138:THR:HG23	1:K:147:VAL:HG13	2.00	0.44
2:B:692:GLY:HA2	2:B:695:TYR:CD2	2.53	0.44
1:C:219:ASP:HB3	1:C:226:HIS:CE1	2.53	0.43
2:F:872:ASP:OD1	2:F:872:ASP:C	2.60	0.43
1:G:84:GLU:HB2	1:G:92:HIS:HB3	2.00	0.43
1:G:394:GLU:HB2	1:G:405:HIS:CE1	2.53	0.43
2:D:638:HIS:O	2:D:669:VAL:HA	2.18	0.43
2:F:667:PRO:HB3	2:F:742:GLN:OE1	2.17	0.43
1:C:203:GLY:O	1:C:204:THR:C	2.61	0.43
1:E:169:LEU:HD13	1:E:175:LEU:HD11	1.99	0.43
1:G:422:PHE:HD2	2:H:612:MET:HE2	1.83	0.43
1:I:211:TYR:CE2	2:J:641:GLY:HA3	2.53	0.43
1:O:199:ARG:NH2	1:O:208:GLU:OE2	2.51	0.43
1:G:220:HIS:ND1	1:G:225:THR:OG1	2.47	0.43
1:K:367:ALA:HB2	1:K:399:VAL:HG21	2.00	0.43
2:L:734:TYR:CZ	2:L:776:ILE:HD12	2.52	0.43
1:M:194:ARG:HD2	1:M:194:ARG:HA	1.84	0.43
2:N:671:PRO:HD2	2:N:695:TYR:CE2	2.54	0.43
1:O:219:ASP:OD1	1:O:221:ARG:HD2	2.19	0.43
2:N:667:PRO:HB3	2:N:742:GLN:OE1	2.19	0.43
1:C:197:TYR:CE1	2:D:597:HIS:CD2	3.06	0.43
2:F:624:ILE:HD12	2:F:639:TRP:HB3	2.01	0.43
2:F:638:HIS:O	2:F:669:VAL:HA	2.19	0.43
1:M:219:ASP:OD1	1:M:221:ARG:HD3	2.18	0.43
1:O:90:ARG:NH2	1:O:117:GLU:OE2	2.48	0.43
1:A:449:ASN:HD22	1:A:454:GLY:H	1.67	0.43
1:C:422:PHE:HD2	2:D:612:MET:CE	2.28	0.43
1:I:361:ILE:HG12	1:I:436:ALA:HB3	2.00	0.43
1:G:197:TYR:CE1	2:H:597:HIS:CD2	3.06	0.43
1:G:422:PHE:CD2	2:H:612:MET:HE2	2.53	0.43
1:M:178:LEU:HD13	1:M:217:TYR:HB3	2.00	0.43
1:G:242:ASN:HD22	1:G:242:ASN:H	1.67	0.43
1:I:365:ASP:HB2	1:I:366:PRO:HD2	2.01	0.43
1:O:333:ILE:HD12	1:O:334:PHE:CE2	2.54	0.43
2:H:519:ASN:HD22	2:H:519:ASN:HA	1.76	0.42
2:H:605:SER:HB3	2:H:636:VAL:HG21	2.01	0.42
2:H:856:VAL:HG11	2:H:888:TYR:CG	2.54	0.42
1:M:327:TYR:HA	1:M:341:PHE:CD1	2.54	0.42
1:A:188:ASN:HB2	1:A:192:TYR:CD1	2.54	0.42
1:G:352:THR:HG21	1:G:486:PHE:CD2	2.54	0.42
2:L:734:TYR:CE2	2:L:776:ILE:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:747:THR:HA	2:L:748:PRO:HD3	1.90	0.42
1:C:422:PHE:CE2	2:D:612:MET:HE3	2.53	0.42
2:D:692:GLY:HA2	2:D:695:TYR:CE2	2.55	0.42
2:F:576:LEU:HB3	2:F:583:THR:HG21	2.01	0.42
2:J:671:PRO:HD2	2:J:695:TYR:CE2	2.53	0.42
2:B:946:ASN:HD22	2:B:947:GLU:N	2.17	0.42
1:I:296:TYR:O	2:J:704:ILE:HA	2.19	0.42
1:K:188:ASN:HB2	1:K:192:TYR:CD1	2.54	0.42
1:G:317:PRO:HB2	2:H:725:ILE:HG21	2.01	0.42
1:M:434:ILE:HD11	2:N:612:MET:HE1	2.01	0.42
2:P:946:ASN:HD22	2:P:947:GLU:H	1.67	0.42
2:F:871:ASP:HB2	2:F:878:GLN:OE1	2.20	0.42
1:I:438:TRP:CD1	2:J:624:ILE:HD11	2.55	0.42
1:M:126:LEU:HG	1:M:263:ALA:HB2	2.02	0.42
1:M:441:MET:HB3	1:M:445:ALA:HB3	2.02	0.42
2:N:633:GLY:HA2	2:N:666:ILE:HG12	2.02	0.42
2:P:872:ASP:C	2:P:872:ASP:OD1	2.62	0.42
1:A:302:TYR:CD2	1:A:478:GLY:HA2	2.55	0.42
1:A:389:GLU:HG2	6:A:504:NAG:C5	2.50	0.42
1:E:458:THR:HG22	1:E:460:GLU:OE1	2.19	0.42
1:I:248:LEU:C	1:I:248:LEU:HD23	2.44	0.42
1:O:169:LEU:HD13	1:O:175:LEU:HD11	2.01	0.42
1:C:439:ILE:HD11	2:D:608:SER:CB	2.49	0.42
1:M:194:ARG:NH2	1:M:195:THR:O	2.53	0.42
2:H:832:ILE:HA	2:H:865:GLU:O	2.20	0.42
2:L:731:LEU:O	2:L:734:TYR:HB3	2.19	0.42
2:B:613:ARG:O	2:B:617:PRO:HA	2.20	0.41
1:I:161:GLN:NE2	2:J:560:HIS:O	2.53	0.41
2:J:808:ARG:NH1	2:J:809:GLY:O	2.53	0.41
2:L:624:ILE:O	2:L:624:ILE:CG2	2.67	0.41
1:G:176:TYR:O	1:G:217:TYR:HA	2.19	0.41
1:G:94:LYS:HD3	1:G:96:LEU:HD22	2.01	0.41
1:I:176:TYR:O	1:I:217:TYR:HA	2.19	0.41
2:H:853:ASN:OD1	2:H:909:THR:HG23	2.19	0.41
1:I:438:TRP:HA	2:J:624:ILE:HD13	2.02	0.41
2:J:946:ASN:HD22	2:J:947:GLU:N	2.18	0.41
1:K:422:PHE:CE2	2:L:612:MET:HE3	2.56	0.41
2:N:652:LEU:HD12	2:N:652:LEU:C	2.45	0.41
1:A:177:GLY:CA	2:B:663:LEU:HD23	2.50	0.41
1:A:443:GLU:N	1:A:444:PRO:CA	2.78	0.41
1:G:365:ASP:HB2	1:G:366:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:399:VAL:CG1	1:I:441:MET:HE3	2.50	0.41
2:D:757:TYR:CE2	2:D:794:PRO:HG2	2.56	0.41
1:G:88:SER:HA	1:G:124:SER:HA	2.01	0.41
1:G:219:ASP:HB3	1:G:226:HIS:CE1	2.55	0.41
1:I:306:ALA:HB3	4:h:1:NAG:H82	2.02	0.41
1:K:219:ASP:HB3	1:K:226:HIS:CE1	2.56	0.41
2:L:519:ASN:HD22	2:L:519:ASN:HA	1.69	0.41
1:C:394:GLU:HB2	1:C:405:HIS:CE1	2.55	0.41
2:H:747:THR:HA	2:H:748:PRO:HD3	1.90	0.41
1:I:443:GLU:N	1:I:444:PRO:CA	2.81	0.41
1:K:449:ASN:HD22	1:K:454:GLY:H	1.68	0.41
1:C:365:ASP:HB2	1:C:366:PRO:HD2	2.02	0.41
2:J:626:ARG:O	2:J:638:HIS:CE1	2.73	0.41
1:M:219:ASP:HB3	1:M:226:HIS:CE1	2.56	0.41
1:M:468:ASP:HA	1:M:469:PRO:HA	1.89	0.41
2:N:747:THR:HA	2:N:748:PRO:HD3	1.92	0.41
1:O:327:TYR:HA	1:O:341:PHE:CD1	2.56	0.41
2:D:747:THR:HA	2:D:748:PRO:HD3	1.93	0.41
2:H:633:GLY:HA2	2:H:666:ILE:HG12	2.03	0.41
2:N:612:MET:HE2	2:N:615:ARG:HD3	2.03	0.41
2:N:789:VAL:HG12	2:N:819:ILE:CD1	2.51	0.41
1:O:415:GLN:HE22	2:P:607:HIS:HA	1.86	0.41
1:A:327:TYR:HA	1:A:341:PHE:CD1	2.56	0.41
2:B:517:ARG:NH2	2:B:618:ASP:OD1	2.46	0.41
2:L:692:GLY:HA2	2:L:695:TYR:CE2	2.56	0.41
1:A:188:ASN:HB2	1:A:192:TYR:CG	2.56	0.40
1:E:217:TYR:CE2	1:E:228:VAL:HB	2.57	0.40
2:J:519:ASN:HD22	2:J:519:ASN:HA	1.68	0.40
1:K:394:GLU:HB2	1:K:405:HIS:CE1	2.56	0.40
2:L:643:ASN:O	2:L:676:PHE:HB3	2.20	0.40
2:L:856:VAL:HG11	2:L:888:TYR:CG	2.56	0.40
1:O:385:ILE:HD12	1:O:385:ILE:C	2.46	0.40
1:C:369:TYR:CZ	1:C:371:LYS:HB2	2.56	0.40
1:G:94:LYS:NZ	1:G:104:GLN:HE22	2.20	0.40
1:K:434:ILE:HD11	2:L:612:MET:HE1	2.03	0.40
2:L:638:HIS:O	2:L:669:VAL:HA	2.22	0.40
1:A:289:LEU:HD13	2:B:735:ILE:HG23	2.04	0.40
1:G:161:GLN:O	1:G:253:ILE:HA	2.21	0.40
1:I:181:HIS:H	2:J:659:GLN:HE22	1.68	0.40
2:J:638:HIS:O	2:J:669:VAL:HA	2.21	0.40
2:P:747:THR:HA	2:P:748:PRO:HD3	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ALA:HB2	1:A:399:VAL:HG21	2.04	0.40
1:C:441:MET:HA	2:D:626:ARG:NH2	2.37	0.40
1:E:363:MET:HE3	1:E:363:MET:HB3	1.98	0.40
1:I:313:THR:O	2:N:937:HIS:HB3	2.21	0.40
1:K:439:ILE:HD11	2:L:608:SER:HB2	2.04	0.40
1:M:449:ASN:HD22	1:M:454:GLY:H	1.70	0.40
1:O:177:GLY:CA	2:P:663:LEU:HD23	2.52	0.40
1:E:365:ASP:HB2	1:E:366:PRO:HD2	2.03	0.40
2:F:740:TYR:O	2:F:743:ASN:HB3	2.22	0.40

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%)	43	55
1	C	463/548 (84%)	440 (95%)	22 (5%)	1 (0%)	43	55
1	E	463/548 (84%)	442 (96%)	20 (4%)	1 (0%)	43	55
1	G	463/548 (84%)	441 (95%)	21 (4%)	1 (0%)	43	55
1	I	463/548 (84%)	446 (96%)	17 (4%)	0	100	100
1	K	463/548 (84%)	442 (96%)	20 (4%)	1 (0%)	43	55
1	M	463/548 (84%)	440 (95%)	22 (5%)	1 (0%)	43	55
1	O	463/548 (84%)	447 (96%)	15 (3%)	1 (0%)	43	55
2	B	434/445 (98%)	413 (95%)	20 (5%)	1 (0%)	43	55
2	D	434/445 (98%)	417 (96%)	16 (4%)	1 (0%)	43	55
2	F	434/445 (98%)	419 (96%)	15 (4%)	0	100	100
2	H	434/445 (98%)	415 (96%)	17 (4%)	2 (0%)	24	31
2	J	434/445 (98%)	418 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	43	55
All	All	7176/7944 (90%)	6861 (96%)	303 (4%)	12 (0%)	43	55

All (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
2	P	807	VAL
1	C	244	ALA
1	O	244	ALA
2	B	645	SER
1	G	399	VAL
2	H	528	PRO
1	K	399	VAL

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%)	53	72
1	C	402/469 (86%)	394 (98%)	8 (2%)	48	67
1	E	402/469 (86%)	395 (98%)	7 (2%)	53	72
1	G	402/469 (86%)	391 (97%)	11 (3%)	39	58
1	I	402/469 (86%)	397 (99%)	5 (1%)	63	79
1	K	402/469 (86%)	396 (98%)	6 (2%)	57	75
1	M	402/469 (86%)	392 (98%)	10 (2%)	42	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	402/469 (86%)	394 (98%)	8 (2%)	48	67
2	B	362/373 (97%)	356 (98%)	6 (2%)	53	72
2	D	362/373 (97%)	354 (98%)	8 (2%)	45	65
2	F	362/373 (97%)	350 (97%)	12 (3%)	33	50
2	H	362/373 (97%)	352 (97%)	10 (3%)	38	56
2	J	362/373 (97%)	349 (96%)	13 (4%)	31	47
2	L	362/373 (97%)	350 (97%)	12 (3%)	33	50
2	N	362/373 (97%)	351 (97%)	11 (3%)	36	53
2	P	362/373 (97%)	351 (97%)	11 (3%)	36	53
All	All	6112/6736 (91%)	5967 (98%)	145 (2%)	43	62

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	194	ARG
1	A	222	GLN
1	A	252	ILE
1	A	371	LYS
1	A	394	GLU
1	A	399	VAL
2	B	583	THR
2	B	639	TRP
2	B	838	ILE
2	B	902	GLU
2	B	932	LYS
2	B	946	ASN
1	C	63	THR
1	C	194	ARG
1	C	222	GLN
1	C	252	ILE
1	C	344	ASN
1	C	371	LYS
1	C	399	VAL
1	C	460	GLU
2	D	535	ARG
2	D	639	TRP
2	D	688	TRP
2	D	783	GLU

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Mol	Chain	Res	Type
2	D	892	LYS
2	D	946	ASN
2	D	948	ILE
2	D	951	LEU
1	E	194	ARG
1	E	222	GLN
1	E	280	THR
1	E	284	THR
1	E	344	ASN
1	E	389	GLU
1	E	399	VAL
2	F	527	SER
2	F	535	ARG
2	F	579	SER
2	F	583	THR
2	F	624	ILE
2	F	639	TRP
2	F	652	LEU
2	F	838	ILE
2	F	902	GLU
2	F	933	LYS
2	F	943	THR
2	F	946	ASN
1	G	161	GLN
1	G	194	ARG
1	G	221	ARG
1	G	242	ASN
1	G	243	ASN
1	G	246	GLN
1	G	252	ILE
1	G	344	ASN
1	G	371	LYS
1	G	389	GLU
1	G	399	VAL
2	H	519	ASN
2	H	526	LYS
2	H	535	ARG
2	H	583	THR
2	H	639	TRP
2	H	810	GLN
2	H	933	LYS
2	H	946	ASN

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Mol	Chain	Res	Type
2	H	948	ILE
2	H	951	LEU
1	I	63	THR
1	I	194	ARG
1	I	252	ILE
1	I	389	GLU
1	I	399	VAL
2	J	519	ASN
2	J	527	SER
2	J	575	THR
2	J	583	THR
2	J	624	ILE
2	J	639	TRP
2	J	688	TRP
2	J	909	THR
2	J	926	GLU
2	J	932	LYS
2	J	946	ASN
2	J	948	ILE
2	J	949	THR
1	K	74	THR
1	K	87	THR
1	K	252	ILE
1	K	344	ASN
1	K	371	LYS
1	K	399	VAL
2	L	519	ASN
2	L	535	ARG
2	L	583	THR
2	L	624	ILE
2	L	639	TRP
2	L	663	LEU
2	L	876	VAL
2	L	916	GLU
2	L	925	VAL
2	L	926	GLU
2	L	946	ASN
2	L	948	ILE
1	M	50	LYS
1	M	62	LEU
1	M	155	LYS
1	M	171	GLN

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Mol	Chain	Res	Type
1	M	178	LEU
1	M	194	ARG
1	M	221	ARG
1	M	344	ASN
1	M	389	GLU
1	M	399	VAL
2	N	519	ASN
2	N	520	LEU
2	N	526	LYS
2	N	560	HIS
2	N	639	TRP
2	N	663	LEU
2	N	713	ARG
2	N	805	LYS
2	N	810	GLN
2	N	946	ASN
2	N	951	LEU
1	O	50	LYS
1	O	161	GLN
1	O	171	GLN
1	O	194	ARG
1	O	221	ARG
1	O	246	GLN
1	O	399	VAL
1	O	450	ARG
2	P	516	SER
2	P	561	LEU
2	P	592	VAL
2	P	639	TRP
2	P	652	LEU
2	P	807	VAL
2	P	838	ILE
2	P	876	VAL
2	P	916	GLU
2	P	946	ASN
2	P	948	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	171	GLN

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Mol	Chain	Res	Type
1	A	172	ASN
1	A	206	GLN
1	A	293	GLN
1	A	299	GLN
1	A	359	HIS
1	A	415	GLN
1	A	430	ASN
1	A	449	ASN
2	B	519	ASN
2	B	560	HIS
2	B	587	GLN
2	B	651	GLN
2	B	723	ASN
2	B	730	GLN
2	B	751	ASN
2	B	759	ASN
2	B	818	ASN
2	B	946	ASN
1	C	104	GLN
1	C	242	ASN
1	C	415	GLN
1	C	430	ASN
1	C	449	ASN
1	C	456	ASN
2	D	569	GLN
2	D	638	HIS
2	D	651	GLN
2	D	723	ASN
2	D	810	GLN
2	D	946	ASN
1	E	104	GLN
1	E	131	GLN
1	E	174	HIS
1	E	234	ASN
1	E	279	GLN
1	E	344	ASN
1	E	415	GLN
1	E	449	ASN
1	E	456	ASN
2	F	519	ASN
2	F	569	GLN
2	F	651	GLN

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Mol	Chain	Res	Type
2	F	659	GLN
1	G	53	GLN
1	G	104	GLN
1	G	131	GLN
1	G	242	ASN
1	G	279	GLN
1	G	396	GLN
1	G	415	GLN
1	G	430	ASN
1	G	449	ASN
1	G	456	ASN
2	H	519	ASN
2	H	524	HIS
2	H	543	GLN
2	H	558	ASN
2	H	560	HIS
2	H	569	GLN
2	H	587	GLN
2	H	651	GLN
2	H	723	ASN
2	H	730	GLN
2	H	759	ASN
2	H	810	GLN
2	H	931	ASN
2	H	946	ASN
1	I	51	HIS
1	I	104	GLN
1	I	206	GLN
1	I	293	GLN
1	I	405	HIS
1	I	415	GLN
1	I	430	ASN
1	I	449	ASN
1	I	456	ASN
1	I	461	ASN
2	J	519	ASN
2	J	539	GLN
2	J	543	GLN
2	J	587	GLN
2	J	593	GLN
2	J	638	HIS
2	J	651	GLN

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Mol	Chain	Res	Type
2	J	659	GLN
2	J	723	ASN
2	J	730	GLN
2	J	818	ASN
2	J	827	HIS
2	J	946	ASN
1	K	104	GLN
1	K	415	GLN
1	K	430	ASN
1	K	449	ASN
1	K	456	ASN
1	K	461	ASN
2	L	519	ASN
2	L	560	HIS
2	L	587	GLN
2	L	607	HIS
2	L	651	GLN
2	L	719	GLN
2	L	723	ASN
2	L	759	ASN
2	L	836	GLN
2	L	946	ASN
1	M	174	HIS
1	M	234	ASN
1	M	344	ASN
1	M	396	GLN
1	M	405	HIS
1	M	415	GLN
1	M	430	ASN
1	M	449	ASN
1	M	456	ASN
2	N	519	ASN
2	N	551	ASN
2	N	558	ASN
2	N	560	HIS
2	N	569	GLN
2	N	587	GLN
2	N	593	GLN
2	N	707	ASN
2	N	723	ASN
2	N	759	ASN
2	N	946	ASN

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Mol	Chain	Res	Type
1	O	171	GLN
1	O	206	GLN
1	O	279	GLN
1	O	415	GLN
1	O	421	GLN
1	O	449	ASN
2	P	519	ASN
2	P	569	GLN
2	P	587	GLN
2	P	651	GLN
2	P	701	HIS
2	P	723	ASN
2	P	730	GLN
2	P	759	ASN
2	P	810	GLN
2	P	946	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	0.74	0
3	GLC	Q	2	3	11,11,12	0.29	0	15,15,17	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	R	1	4,1	14,14,15	0.35	0	17,19,21	0.64	1 (5%)
4	NAG	R	2	4	14,14,15	0.31	0	17,19,21	0.80	1 (5%)
3	GLC	S	1	3	12,12,12	0.54	0	17,17,17	0.62	0
3	GLC	S	2	3	11,11,12	0.29	0	15,15,17	0.54	0
5	NAG	T	1	5,2	14,14,15	0.52	0	17,19,21	0.97	0
5	NAG	T	2	5	14,14,15	0.37	0	17,19,21	0.79	0
5	BMA	T	3	5	11,11,12	0.38	0	15,15,17	0.76	0
3	GLC	U	1	3	12,12,12	0.55	0	17,17,17	0.66	0
3	GLC	U	2	3	11,11,12	0.29	0	15,15,17	0.53	0
4	NAG	V	1	4,1	14,14,15	0.41	0	17,19,21	0.97	0
4	NAG	V	2	4	14,14,15	0.50	0	17,19,21	1.14	1 (5%)
3	GLC	W	1	3	12,12,12	0.50	0	17,17,17	0.75	1 (5%)
3	GLC	W	2	3	11,11,12	0.36	0	15,15,17	1.01	1 (6%)
5	NAG	X	1	5,2	14,14,15	0.57	0	17,19,21	1.18	2 (11%)
5	NAG	X	2	5	14,14,15	0.41	0	17,19,21	1.28	2 (11%)
5	BMA	X	3	5	11,11,12	0.41	0	15,15,17	1.25	1 (6%)
3	GLC	Y	1	3	12,12,12	0.56	0	17,17,17	0.72	0
3	GLC	Y	2	3	11,11,12	0.27	0	15,15,17	0.64	0
4	NAG	Z	1	4,1	14,14,15	0.38	0	17,19,21	0.56	0
4	NAG	Z	2	4	14,14,15	0.43	0	17,19,21	0.84	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	0.28	0	15,15,17	0.58	0
5	NAG	b	1	5,2	14,14,15	0.55	0	17,19,21	0.93	1 (5%)
5	NAG	b	2	5	14,14,15	0.47	0	17,19,21	1.82	3 (17%)
5	BMA	b	3	5	11,11,12	0.42	0	15,15,17	0.90	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	0.43	0
4	NAG	d	1	4,1	14,14,15	0.40	0	17,19,21	0.78	1 (5%)
4	NAG	d	2	4	14,14,15	0.43	0	17,19,21	0.87	1 (5%)
3	GLC	e	1	3	12,12,12	0.51	0	17,17,17	0.72	0
3	GLC	e	2	3	11,11,12	0.36	0	15,15,17	0.46	0
5	NAG	f	1	5,2	14,14,15	0.60	0	17,19,21	0.89	1 (5%)
5	NAG	f	2	5	14,14,15	0.49	0	17,19,21	1.68	4 (23%)
5	BMA	f	3	5	11,11,12	0.41	0	15,15,17	0.83	0
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	0.25	0	15,15,17	0.73	0
4	NAG	h	1	4,1	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
4	NAG	h	2	4	14,14,15	0.45	0	17,19,21	1.03	1 (5%)
3	GLC	i	1	3	12,12,12	0.60	0	17,17,17	1.22	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	i	2	3	11,11,12	0.30	0	15,15,17	0.69	0
5	NAG	j	1	5,2	14,14,15	0.43	0	17,19,21	0.73	0
5	NAG	j	2	5	14,14,15	0.44	0	17,19,21	1.21	2 (11%)
5	BMA	j	3	5	11,11,12	0.38	0	15,15,17	0.86	0
3	GLC	k	1	3	12,12,12	0.45	0	17,17,17	0.85	0
3	GLC	k	2	3	11,11,12	0.31	0	15,15,17	0.57	0
4	NAG	l	1	4,1	14,14,15	0.40	0	17,19,21	0.78	0
4	NAG	l	2	4	14,14,15	0.35	0	17,19,21	1.08	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	0.49	0
5	NAG	n	1	5,2	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
5	NAG	n	2	5	14,14,15	0.36	0	17,19,21	1.15	2 (11%)
5	BMA	n	3	5	11,11,12	0.41	0	15,15,17	0.86	0
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	0.71	0
4	NAG	p	1	4,1	14,14,15	0.40	0	17,19,21	0.85	0
4	NAG	p	2	4	14,14,15	0.34	0	17,19,21	1.06	1 (5%)
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	0.67	0
5	NAG	r	1	5,2	14,14,15	0.43	0	17,19,21	1.63	4 (23%)
5	NAG	r	2	5	14,14,15	0.37	0	17,19,21	1.09	2 (11%)
5	BMA	r	3	5	11,11,12	0.40	0	15,15,17	0.84	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	0.31	0	15,15,17	0.60	0
4	NAG	t	1	4,1	14,14,15	0.36	0	17,19,21	0.91	1 (5%)
4	NAG	t	2	4	14,14,15	0.37	0	17,19,21	1.09	1 (5%)
3	GLC	u	1	3	12,12,12	0.58	0	17,17,17	0.71	0
3	GLC	u	2	3	11,11,12	0.27	0	15,15,17	0.56	0
5	NAG	v	1	5,2	14,14,15	0.50	0	17,19,21	1.06	1 (5%)
5	NAG	v	2	5	14,14,15	0.39	0	17,19,21	0.99	0
5	BMA	v	3	5	11,11,12	0.38	0	15,15,17	0.80	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	R	1	4,1	-	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	-	4/6/23/26	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	4,1	-	1/6/23/26	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	4,1	-	0/6/23/26	0/1/1/1
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	4,1	-	1/6/23/26	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	-	3/6/23/26	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	4,1	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	i	2	3	-	0/2/19/22	0/1/1/1
5	NAG	j	1	5,2	-	2/6/23/26	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	4,1	-	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	-	3/6/23/26	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	4,1	-	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
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	4,1	-	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	-	3/6/23/26	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.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	2	NAG	C1-O5-C5	5.35	119.36	112.19
5	r	1	NAG	C2-N2-C7	4.29	128.65	122.90
5	f	2	NAG	C4-C3-C2	4.06	116.97	111.02
4	t	2	NAG	C1-O5-C5	3.63	117.05	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	l	2	NAG	C1-O5-C5	3.47	116.83	112.19
5	X	3	BMA	C3-C4-C5	3.19	116.01	110.23
5	v	1	NAG	C1-O5-C5	3.10	116.34	112.19
4	t	1	NAG	C1-O5-C5	3.06	116.29	112.19
5	r	1	NAG	C1-C2-N2	3.02	115.20	110.43
5	f	2	NAG	C1-O5-C5	2.90	116.08	112.19
5	f	2	NAG	C3-C4-C5	2.84	115.39	110.23
4	p	2	NAG	C1-O5-C5	2.78	115.91	112.19
5	b	2	NAG	O5-C5-C4	2.72	117.45	110.83
4	h	1	NAG	O5-C1-C2	-2.69	107.12	111.29
3	i	1	GLC	C4-C3-C2	2.66	115.50	110.83
3	i	1	GLC	C1-C2-C3	2.61	115.69	110.36
5	X	2	NAG	C1-O5-C5	2.59	115.66	112.19
5	j	2	NAG	C4-C3-C2	2.59	114.81	111.02
5	n	2	NAG	C1-O5-C5	2.56	115.61	112.19
3	W	2	GLC	C3-C4-C5	2.48	114.74	110.23
4	h	2	NAG	C1-O5-C5	2.48	115.51	112.19
5	f	2	NAG	C1-C2-N2	-2.48	106.53	110.43
5	X	2	NAG	O5-C1-C2	-2.47	107.47	111.29
5	j	2	NAG	C1-O5-C5	2.45	115.46	112.19
5	b	2	NAG	C3-C4-C5	2.40	114.58	110.23
3	W	1	GLC	O5-C5-C6	2.34	112.23	106.44
4	V	2	NAG	O5-C5-C4	-2.33	105.16	110.83
5	r	2	NAG	C1-O5-C5	2.30	115.26	112.19
5	b	1	NAG	C2-N2-C7	2.25	125.91	122.90
5	b	3	BMA	C1-O5-C5	2.17	115.10	112.19
5	X	1	NAG	O5-C1-C2	-2.15	107.97	111.29
5	n	1	NAG	O5-C1-C2	-2.12	108.00	111.29
5	r	1	NAG	C4-C3-C2	2.12	114.12	111.02
4	d	1	NAG	C1-O5-C5	2.11	115.01	112.19
4	d	2	NAG	C1-C2-N2	-2.11	107.11	110.43
5	X	1	NAG	O4-C4-C5	-2.09	104.18	109.32
5	n	2	NAG	O5-C1-C2	-2.09	108.06	111.29
4	R	2	NAG	C1-O5-C5	2.07	114.96	112.19
5	r	2	NAG	C4-C3-C2	2.05	114.02	111.02
4	R	1	NAG	O5-C1-C2	-2.04	108.13	111.29
5	f	1	NAG	O5-C1-C2	-2.03	108.16	111.29
5	r	1	NAG	O5-C1-C2	-2.01	108.18	111.29

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	r	1	NAG	C1-C2-N2-C7
5	r	3	BMA	O5-C5-C6-O6
3	W	2	GLC	C4-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
5	b	3	BMA	O5-C5-C6-O6
5	n	3	BMA	O5-C5-C6-O6
5	X	3	BMA	C4-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
5	j	3	BMA	C4-C5-C6-O6
5	b	3	BMA	C4-C5-C6-O6
5	n	3	BMA	C4-C5-C6-O6
5	r	3	BMA	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
5	f	3	BMA	O5-C5-C6-O6
3	W	2	GLC	O5-C5-C6-O6
5	v	3	BMA	O5-C5-C6-O6
5	T	3	BMA	C4-C5-C6-O6
5	v	3	BMA	C4-C5-C6-O6
5	f	3	BMA	C4-C5-C6-O6
3	W	1	GLC	O5-C5-C6-O6
5	j	3	BMA	O5-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	v	2	NAG	C4-C5-C6-O6
5	v	2	NAG	O5-C5-C6-O6
5	n	2	NAG	O5-C5-C6-O6
3	W	1	GLC	C4-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	n	1	NAG	O5-C5-C6-O6
5	r	2	NAG	O5-C5-C6-O6
5	X	1	NAG	C3-C2-N2-C7
5	X	2	NAG	C4-C5-C6-O6
5	f	1	NAG	O5-C5-C6-O6
5	j	2	NAG	C4-C5-C6-O6
5	T	1	NAG	C3-C2-N2-C7
5	b	1	NAG	C3-C2-N2-C7
5	j	1	NAG	C3-C2-N2-C7
5	v	1	NAG	O5-C5-C6-O6
4	V	1	NAG	C1-C2-N2-C7
4	d	1	NAG	C1-C2-N2-C7
5	T	1	NAG	C1-C2-N2-C7
5	f	1	NAG	C1-C2-N2-C7

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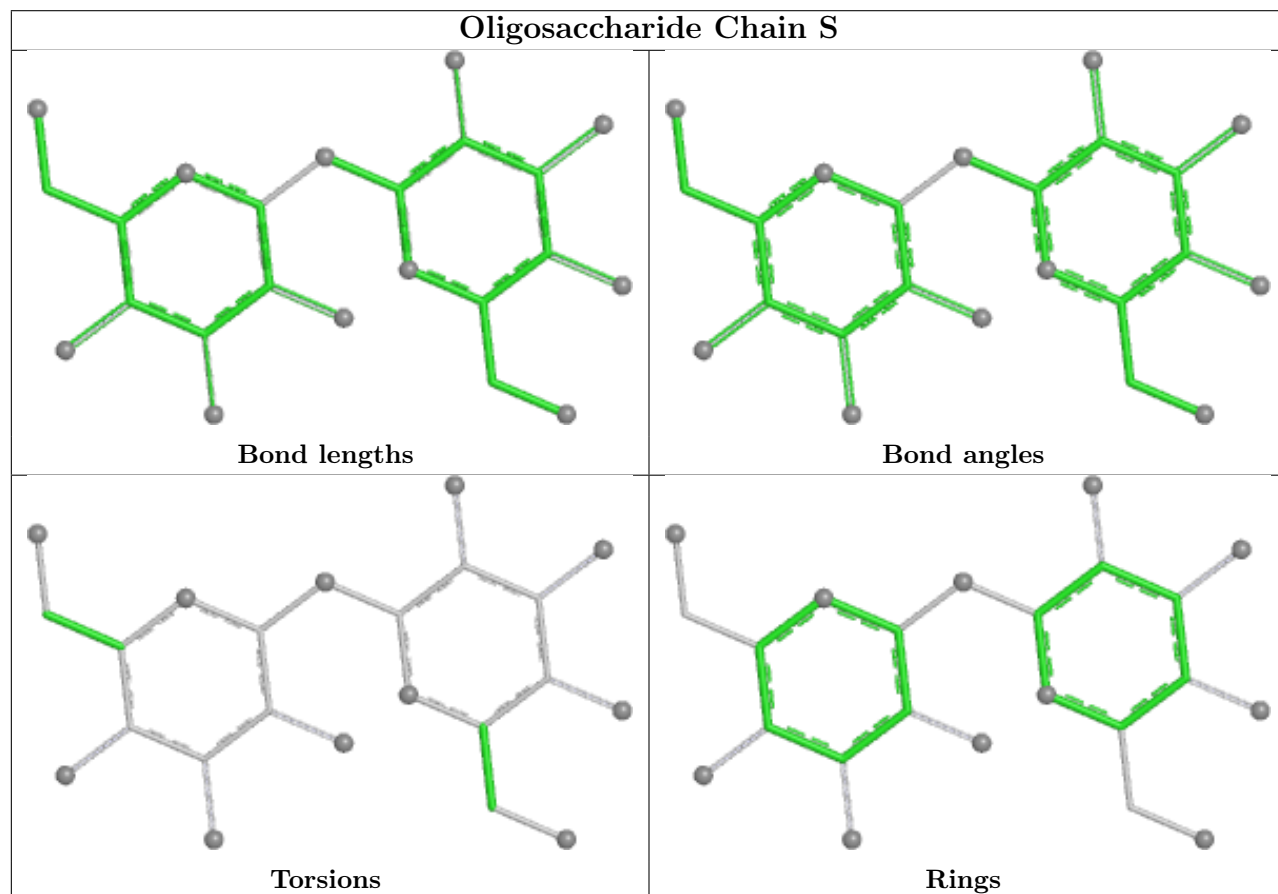
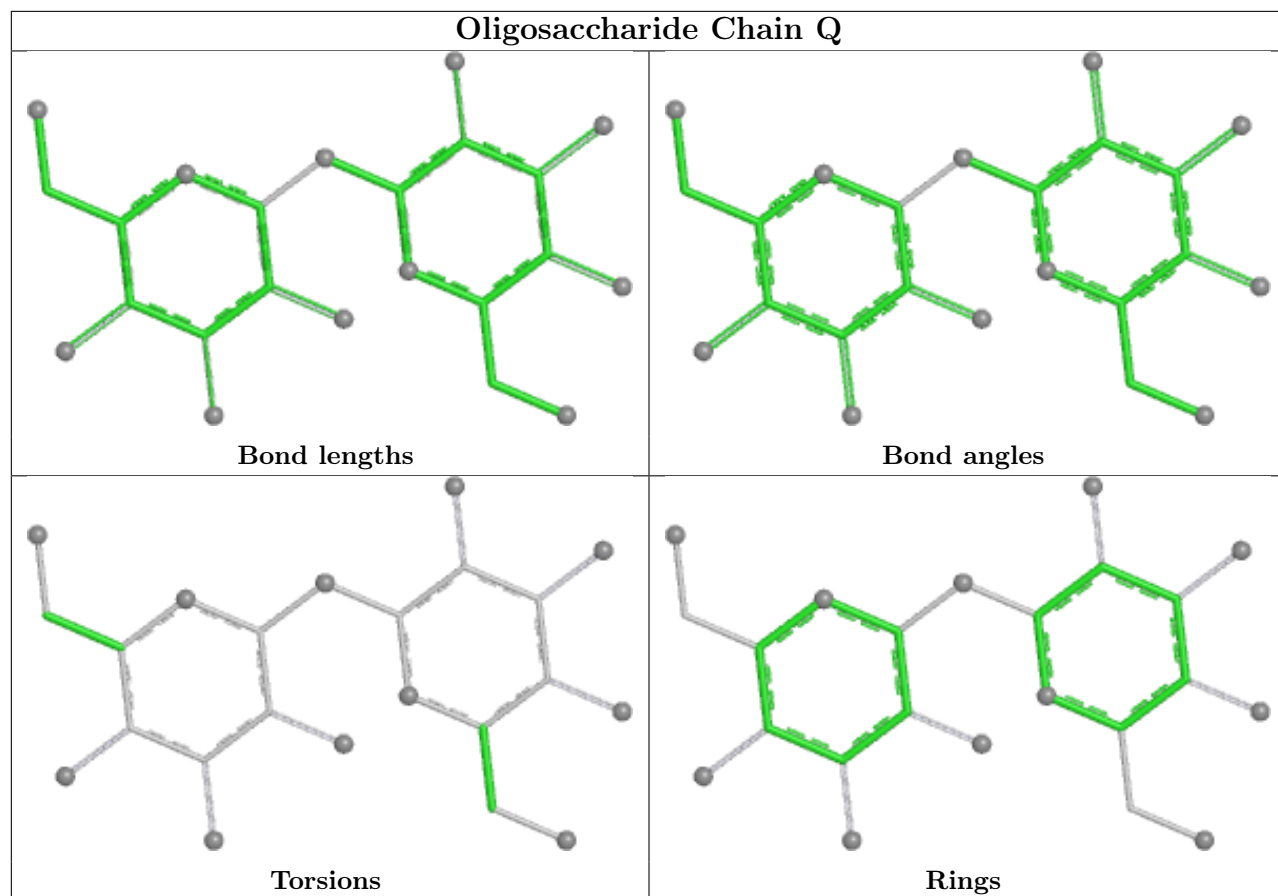
Mol	Chain	Res	Type	Atoms
5	j	1	NAG	C1-C2-N2-C7
5	n	1	NAG	C1-C2-N2-C7
5	v	1	NAG	C1-C2-N2-C7
5	b	1	NAG	O5-C5-C6-O6
5	f	1	NAG	C3-C2-N2-C7
5	n	1	NAG	C3-C2-N2-C7
5	v	1	NAG	C3-C2-N2-C7
3	e	1	GLC	O5-C5-C6-O6
5	n	2	NAG	C4-C5-C6-O6
5	j	2	NAG	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6

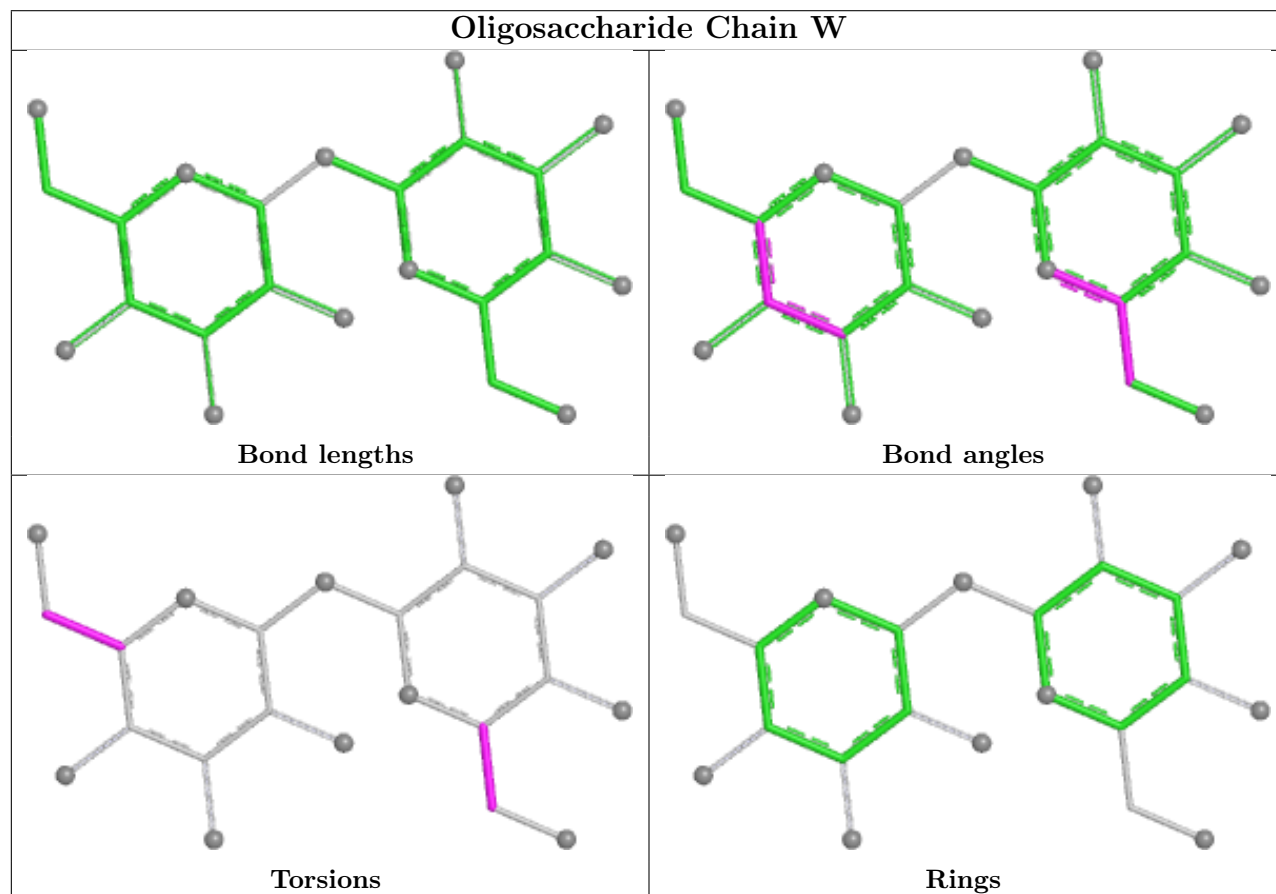
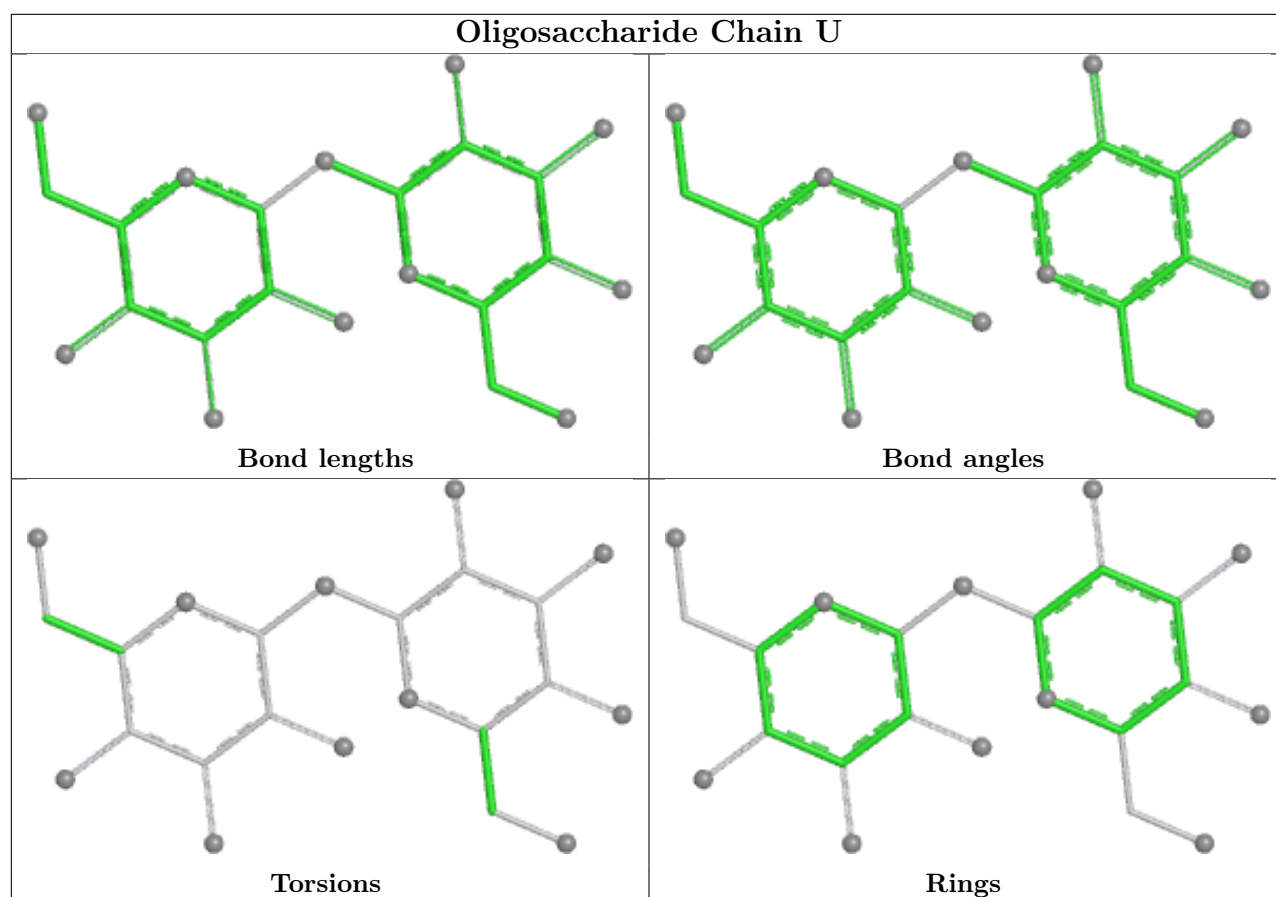
There are no ring outliers.

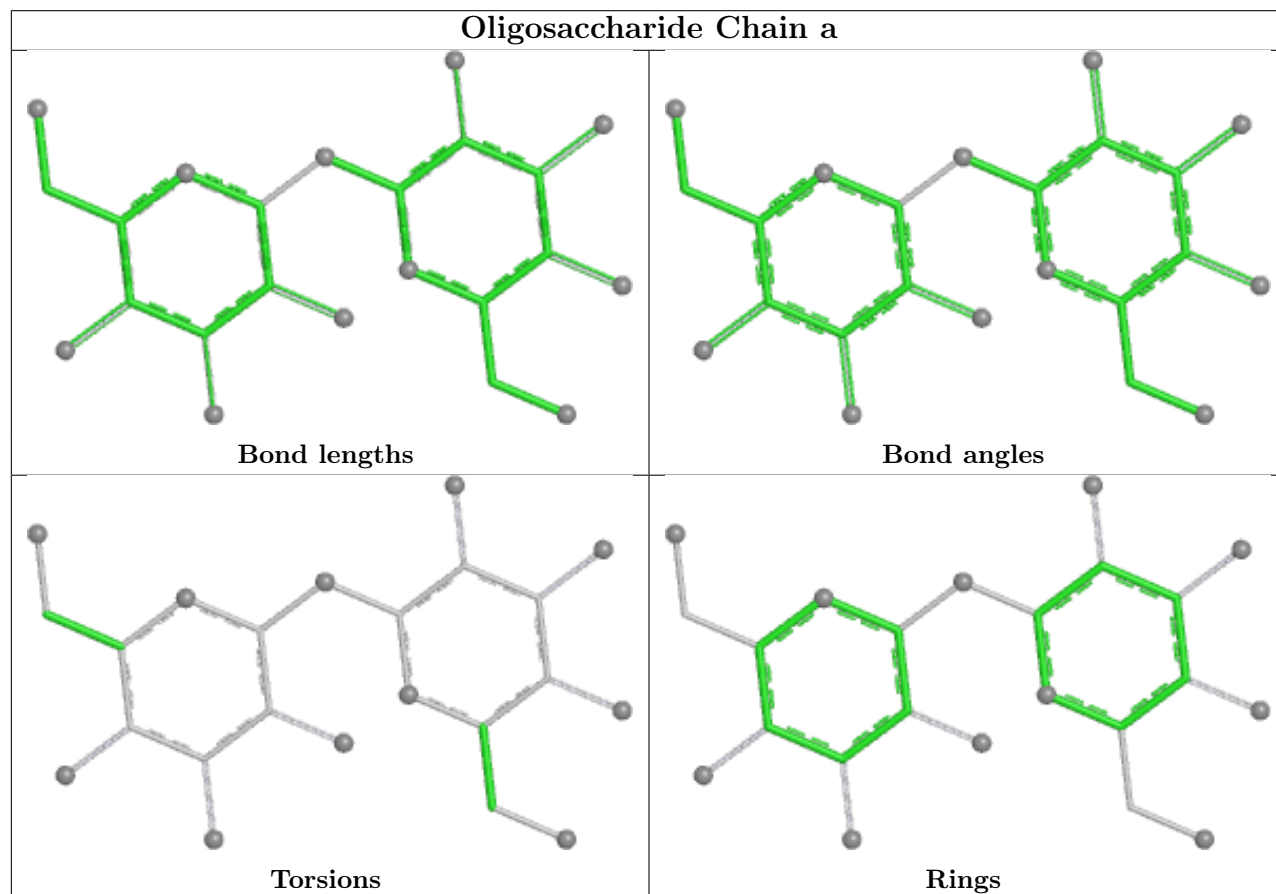
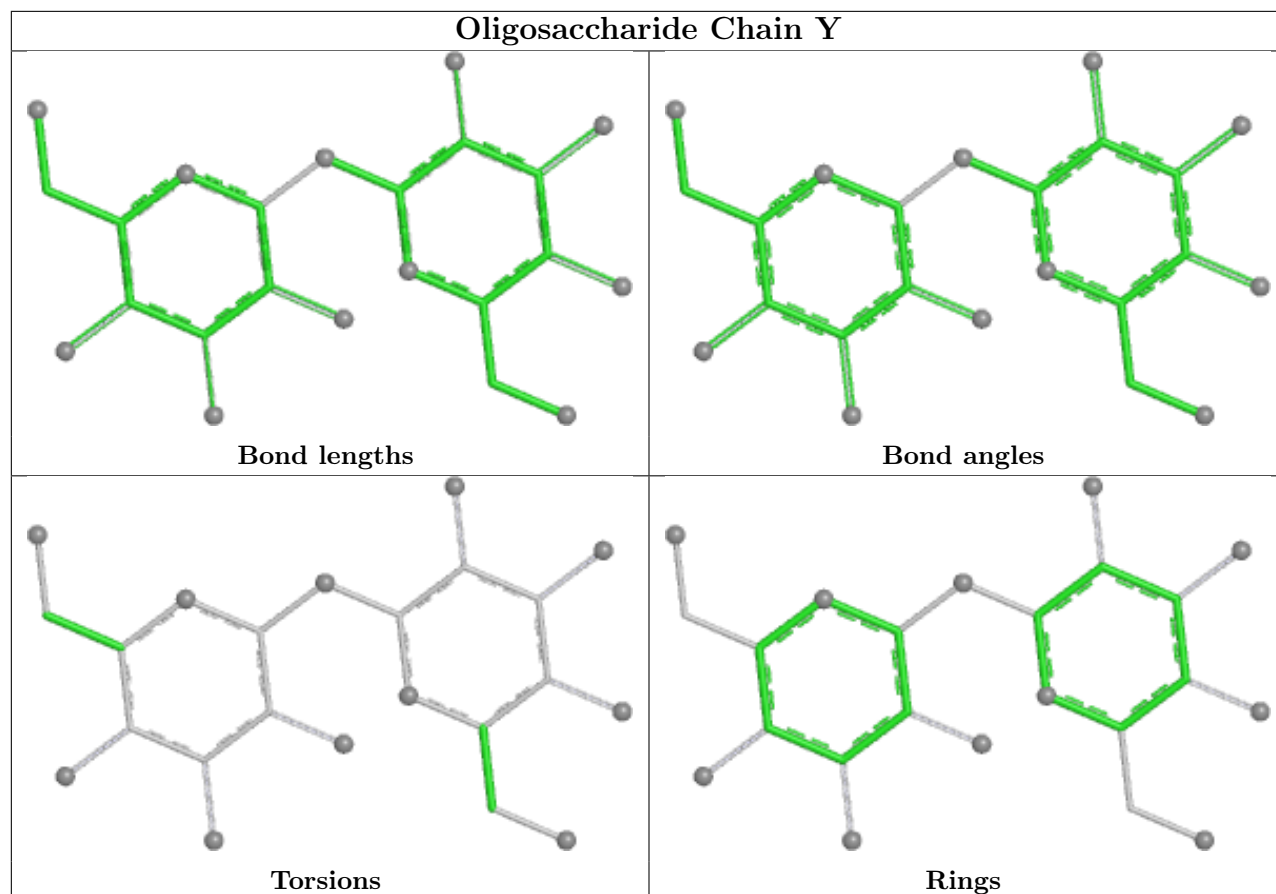
5 monomers are involved in 5 short contacts:

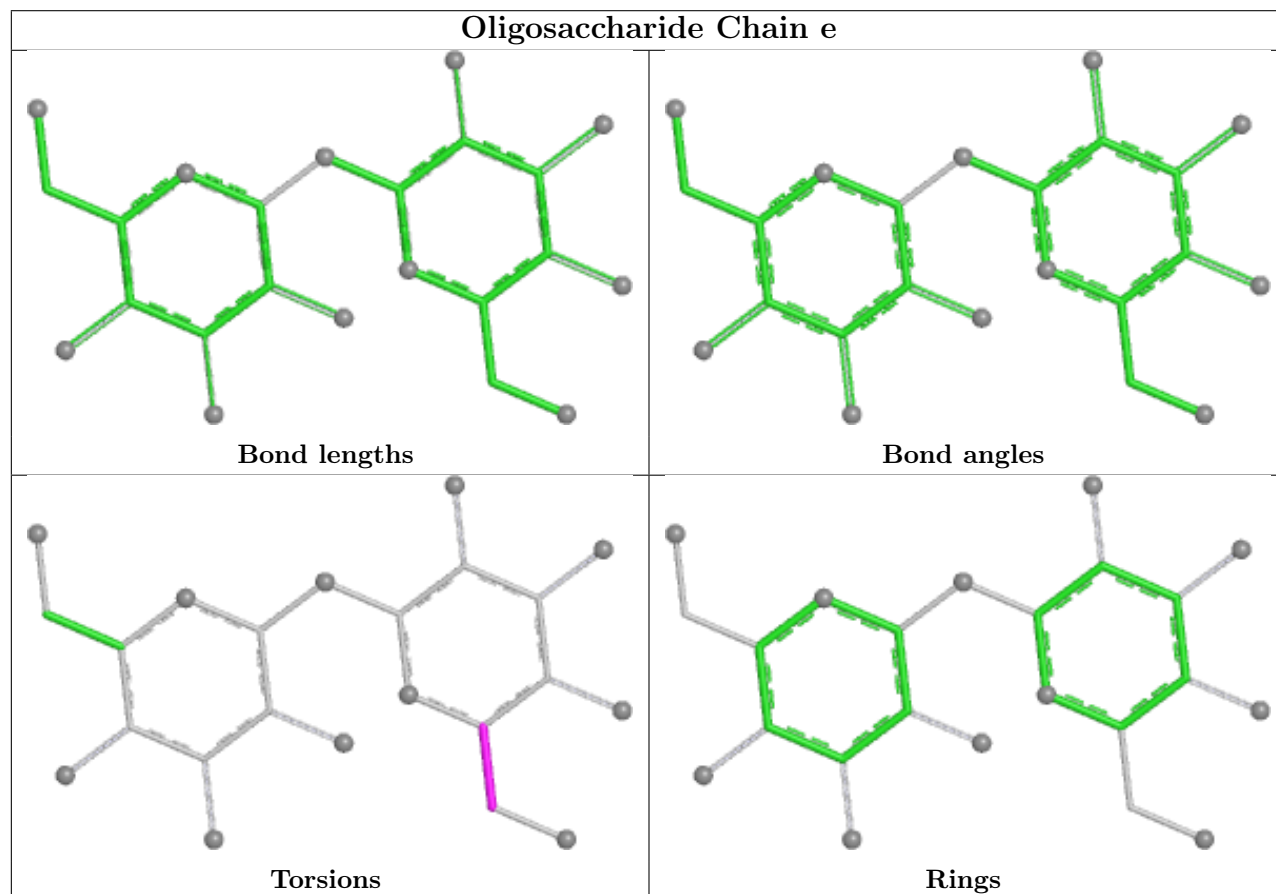
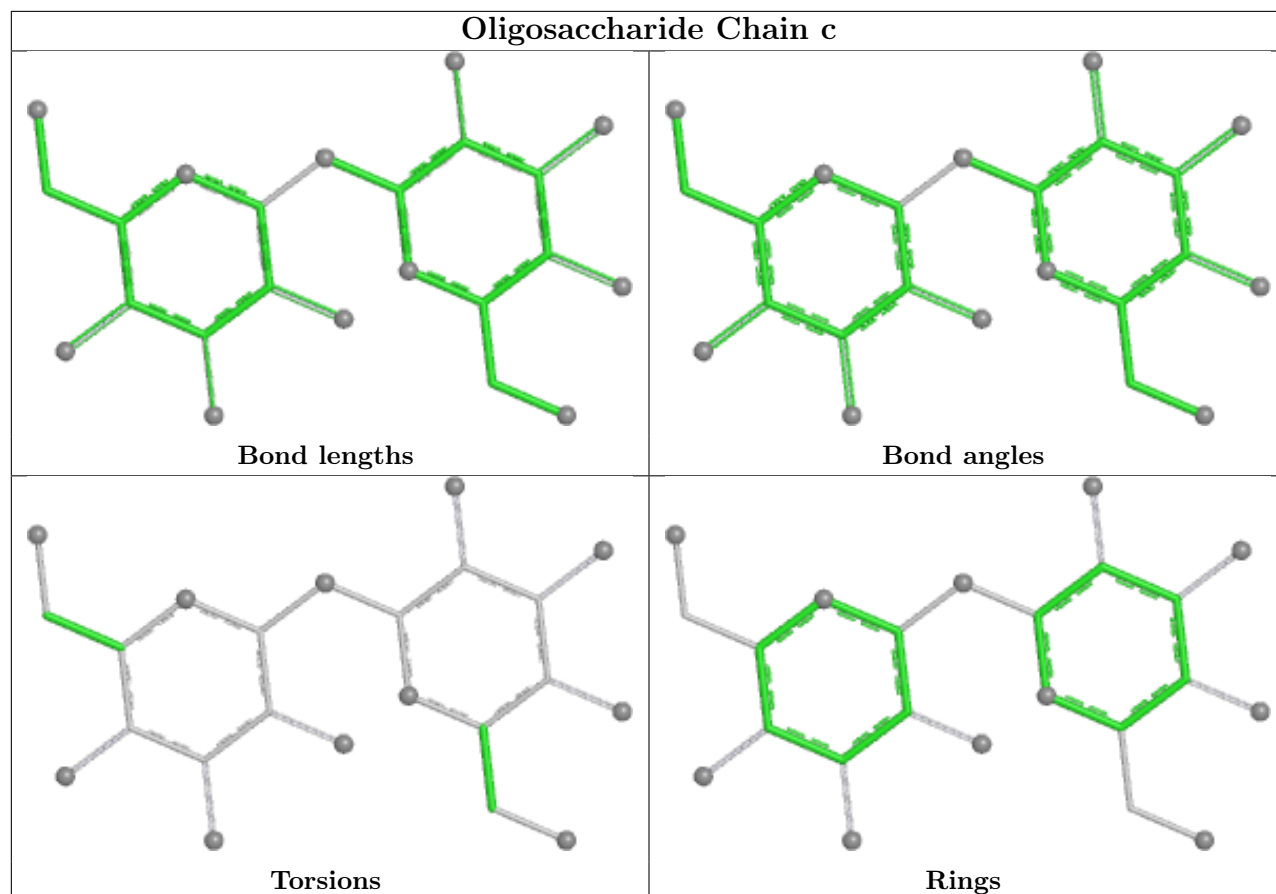
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	3	BMA	1	0
4	d	1	NAG	1	0
4	h	1	NAG	1	0
5	T	2	NAG	1	0
5	b	1	NAG	2	0

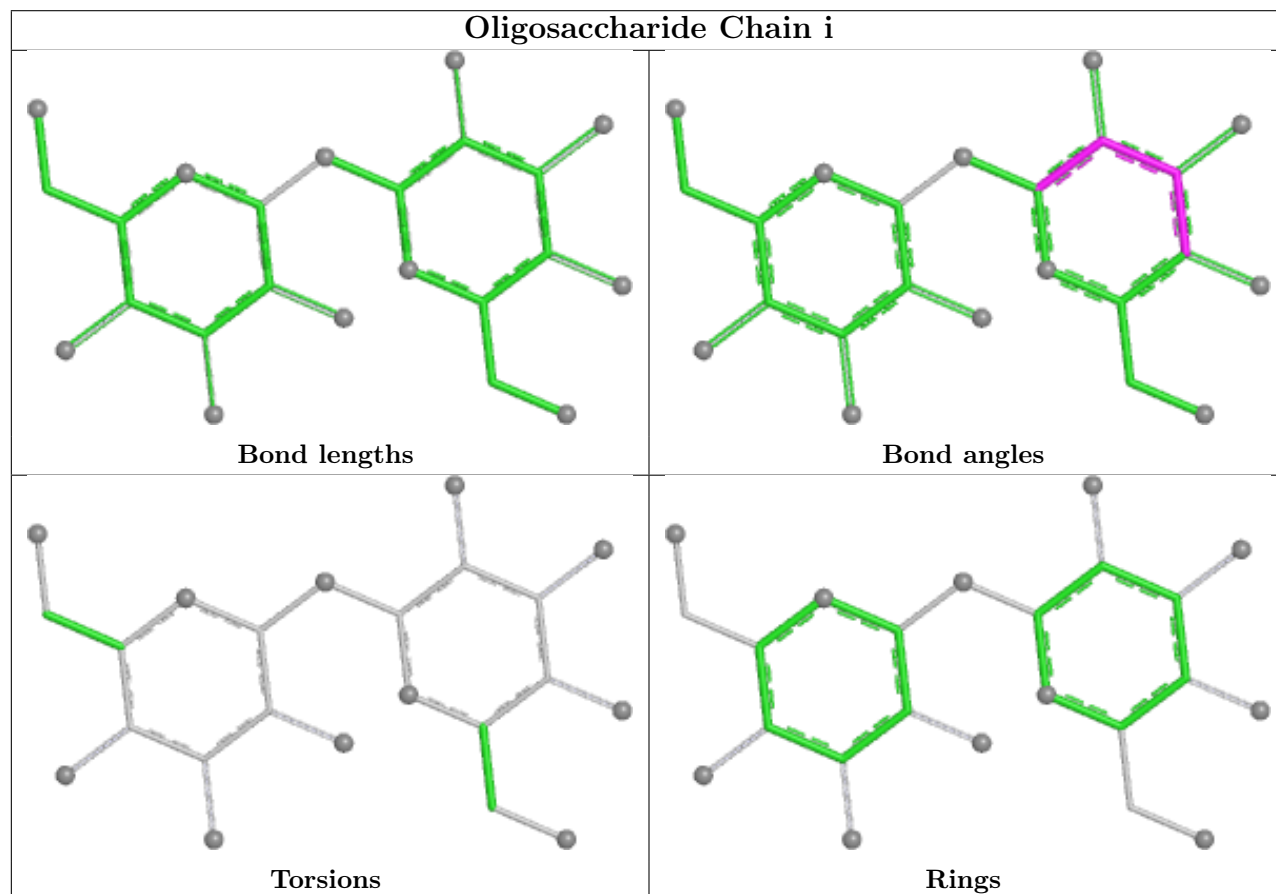
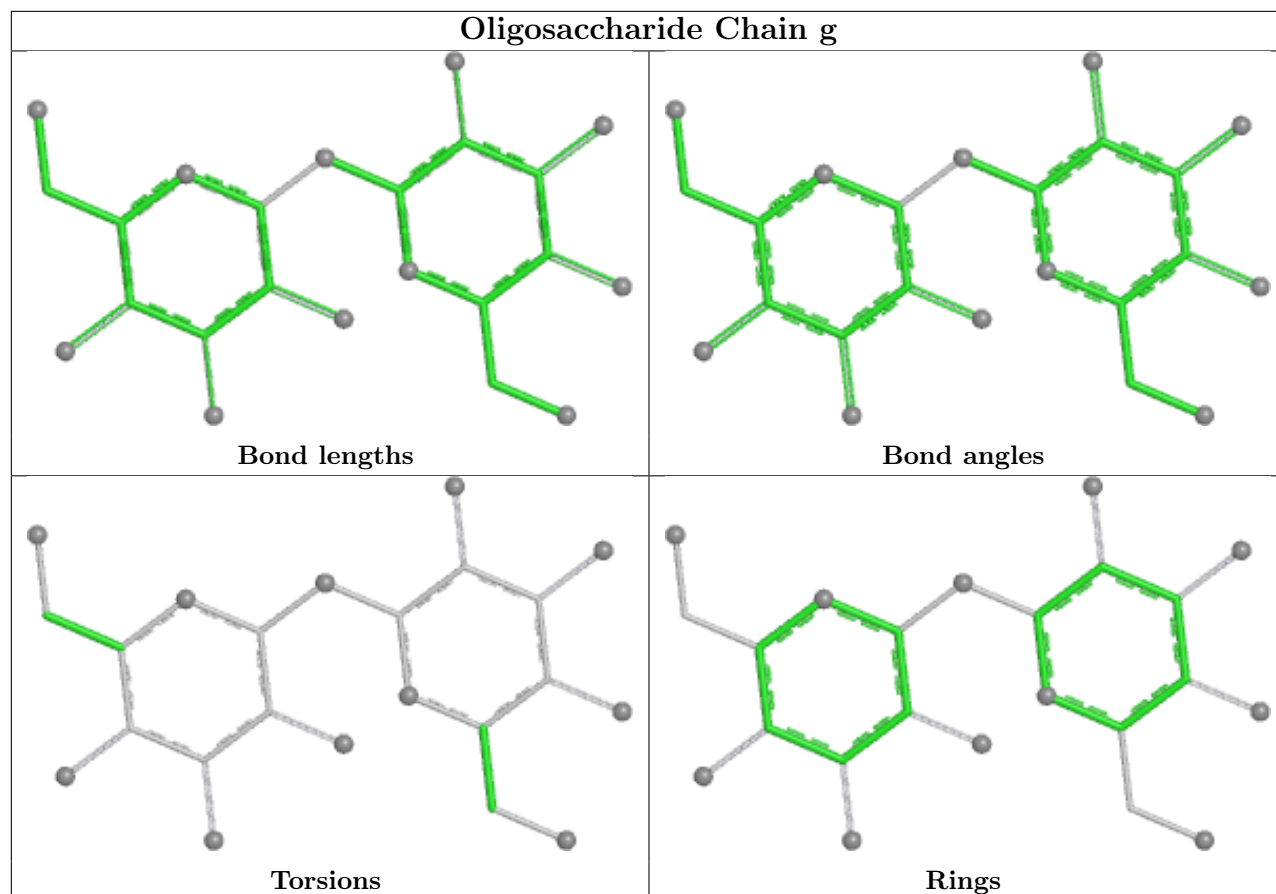
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

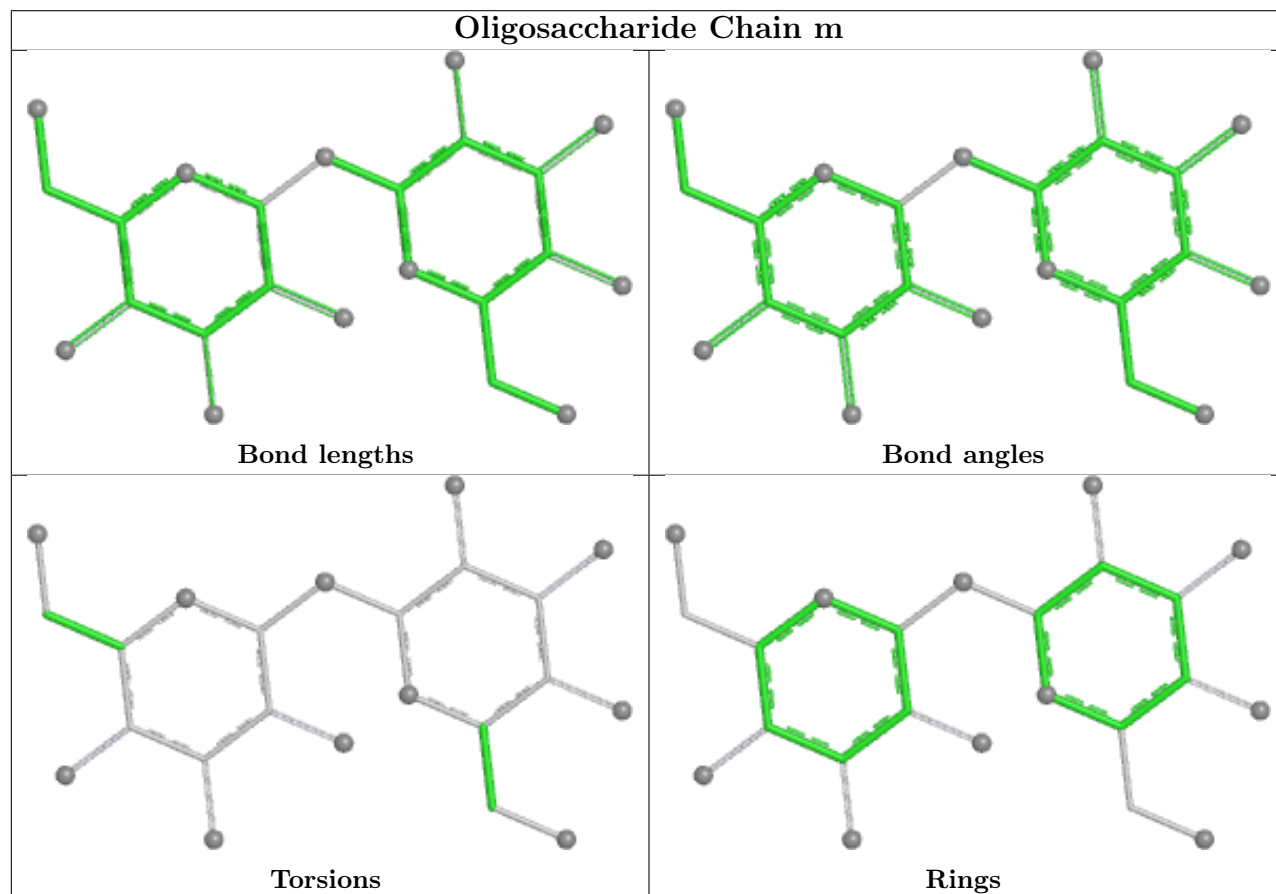
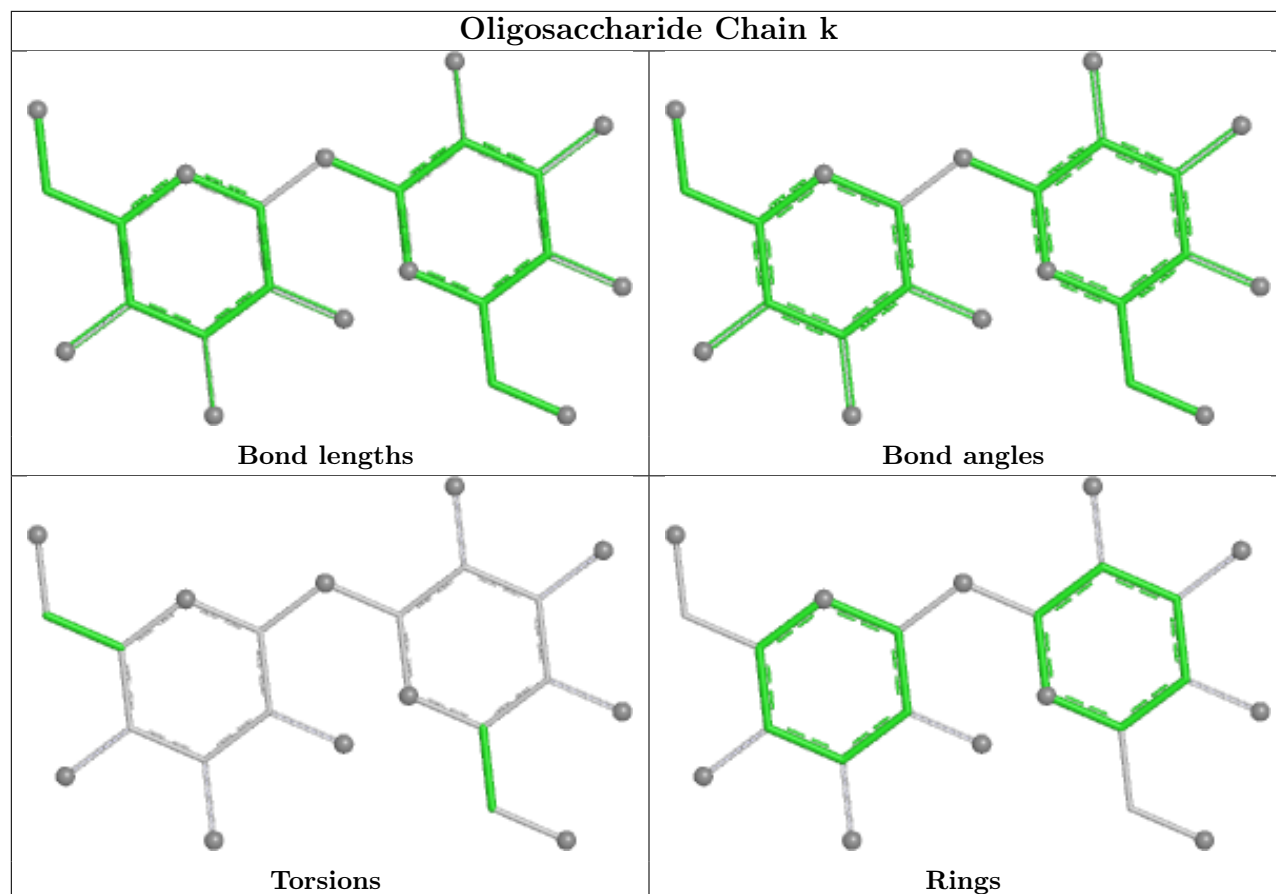


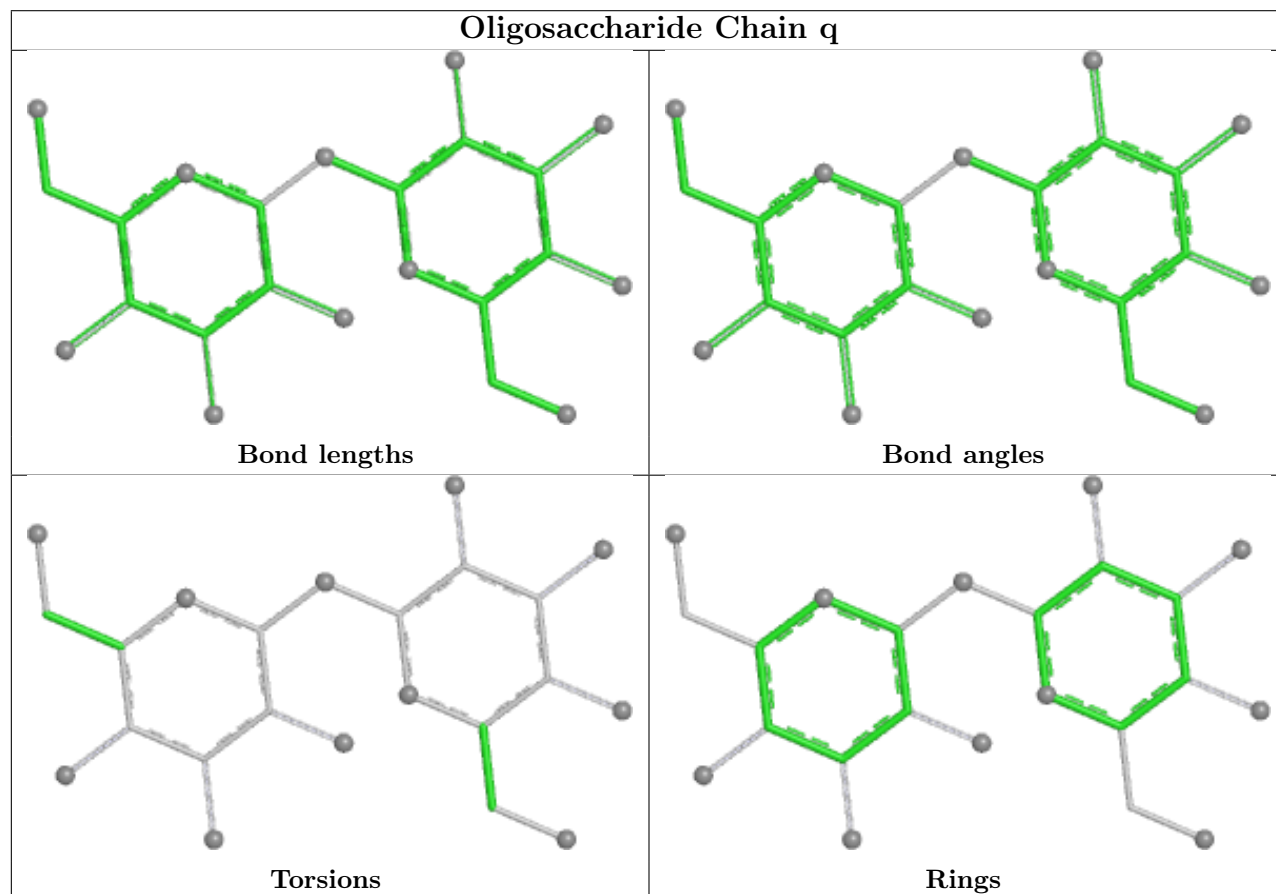
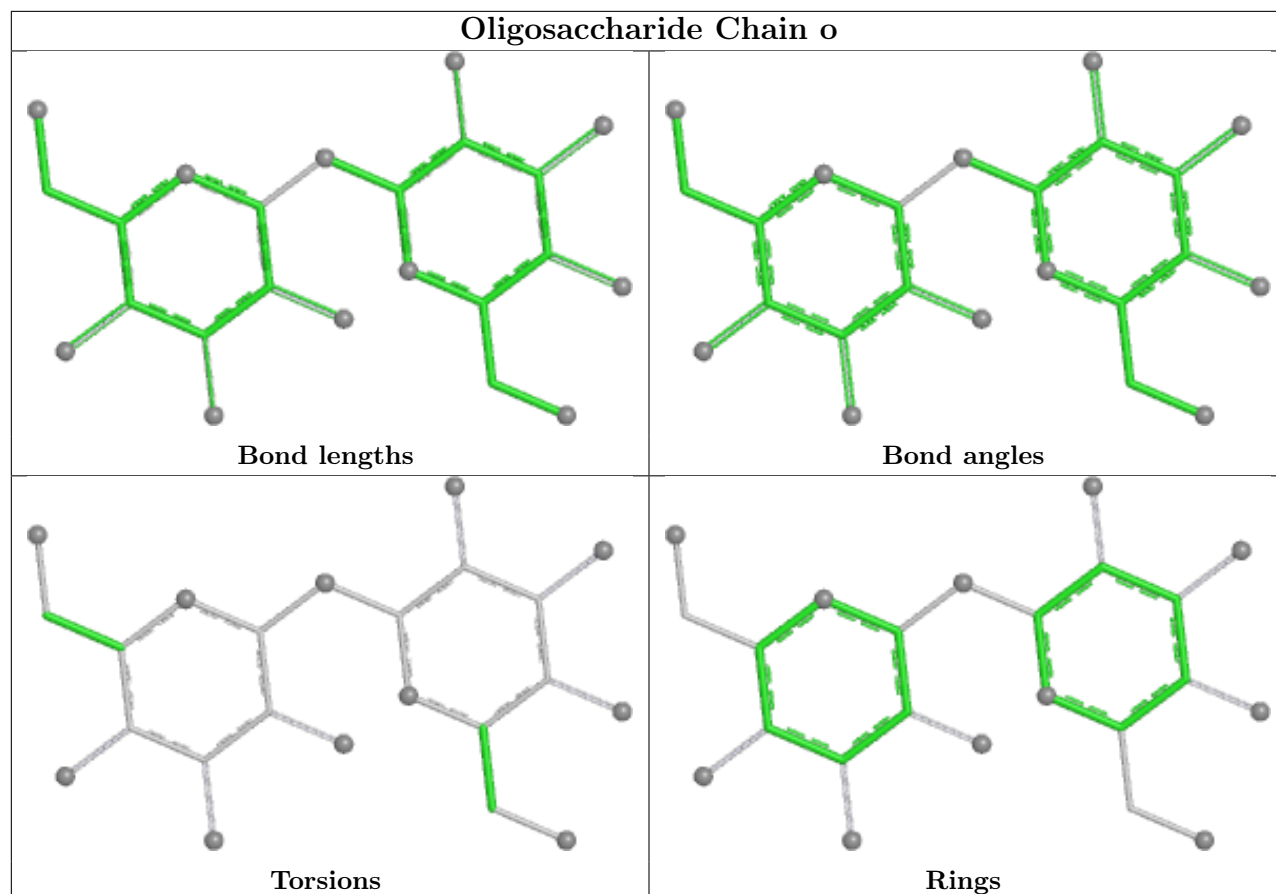


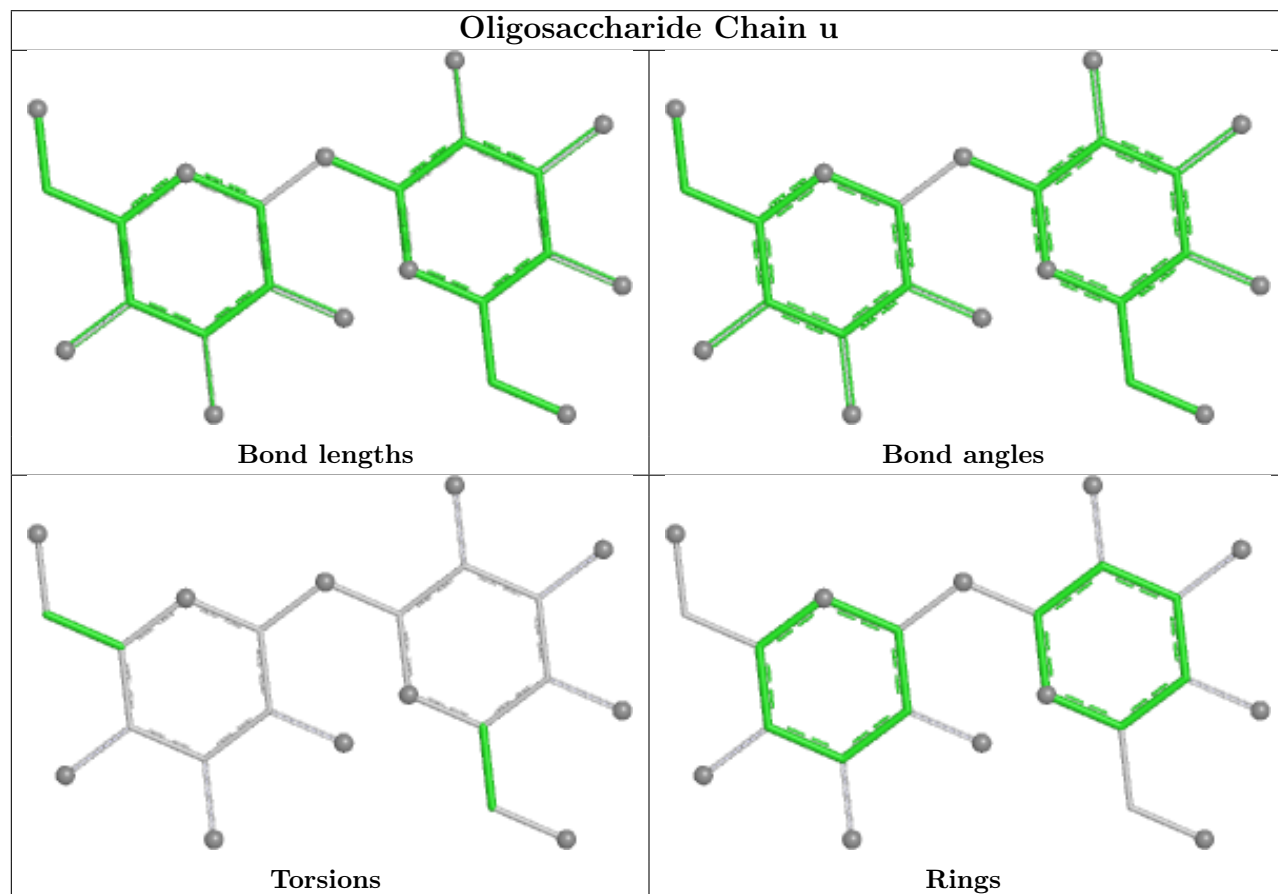
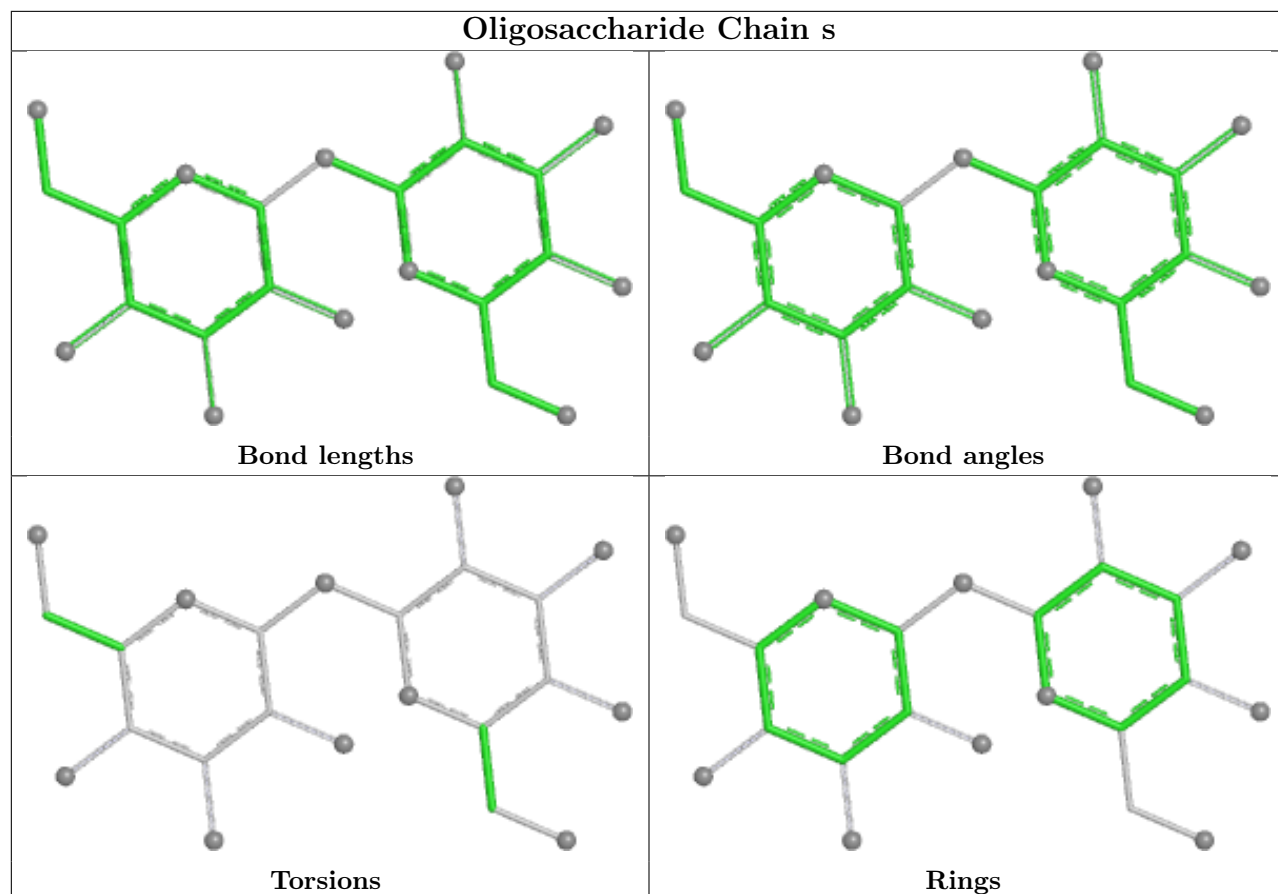


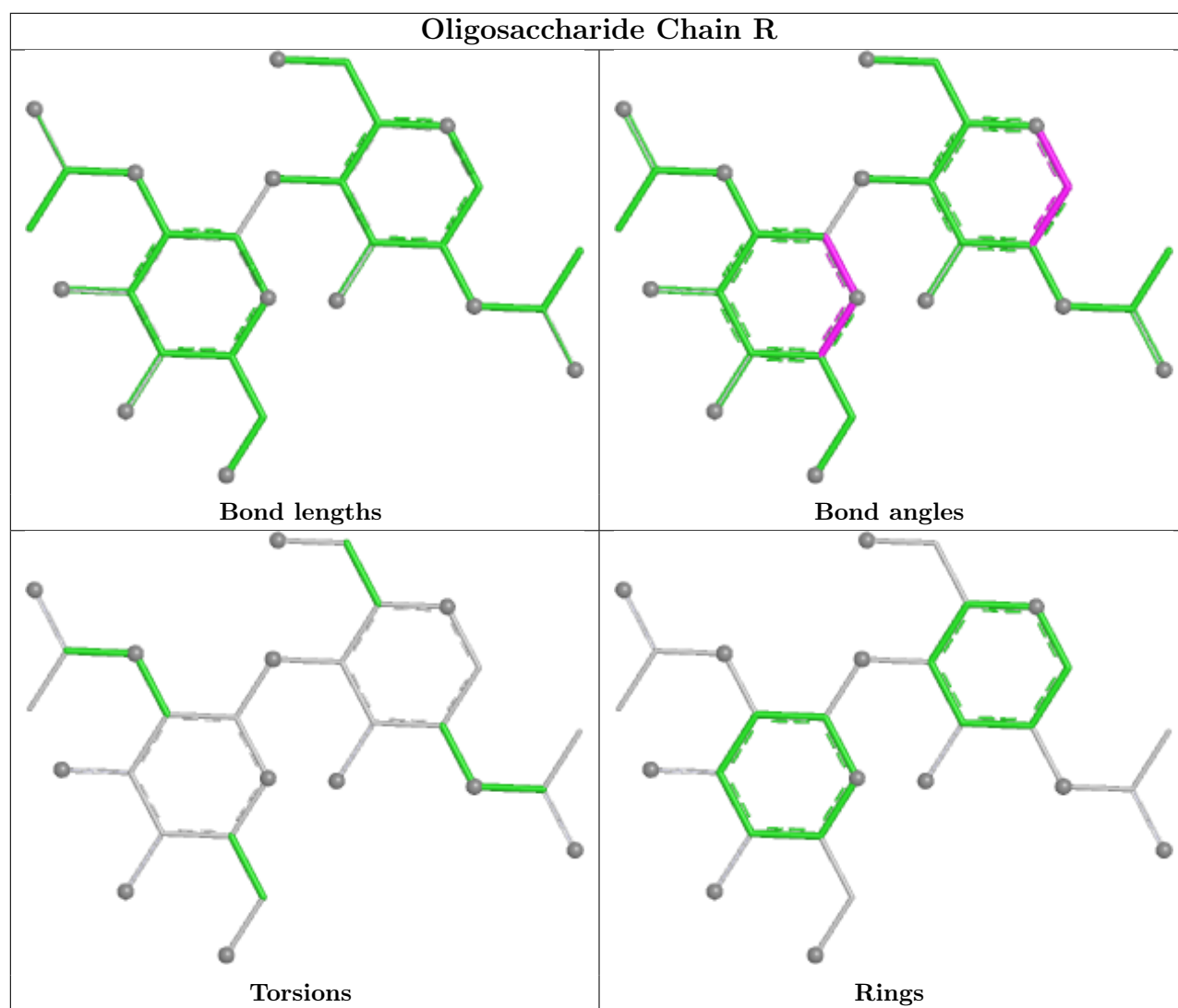


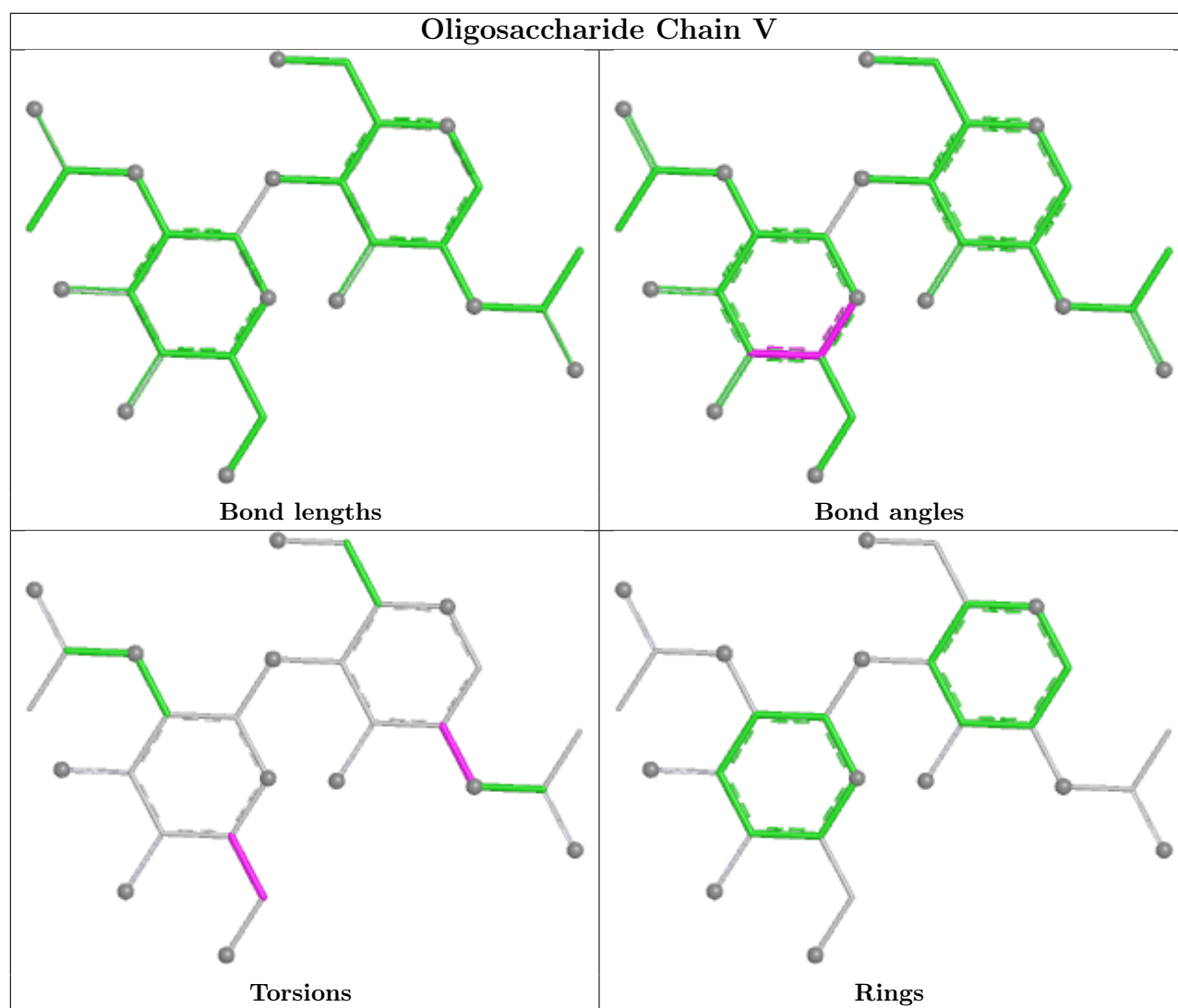


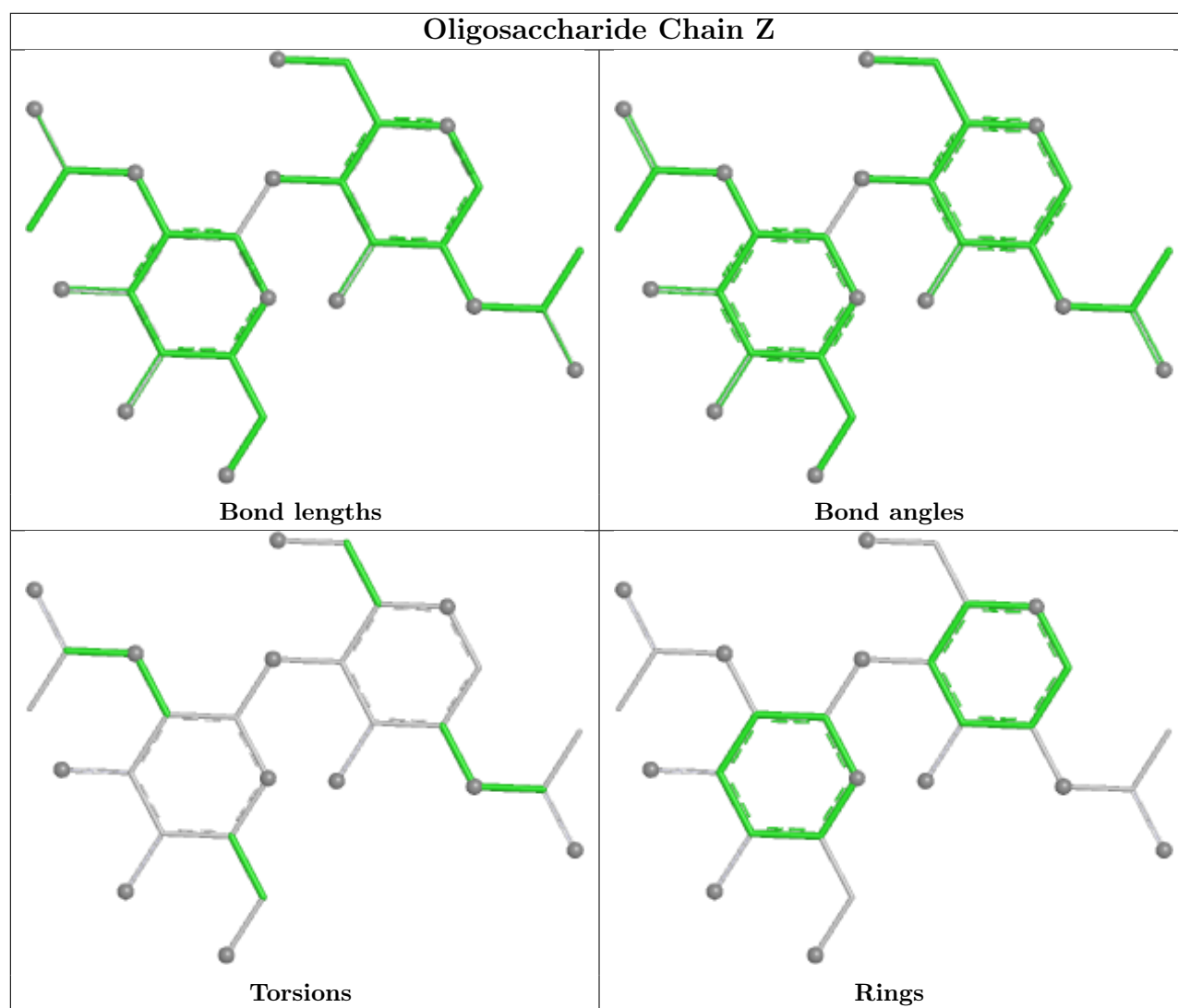


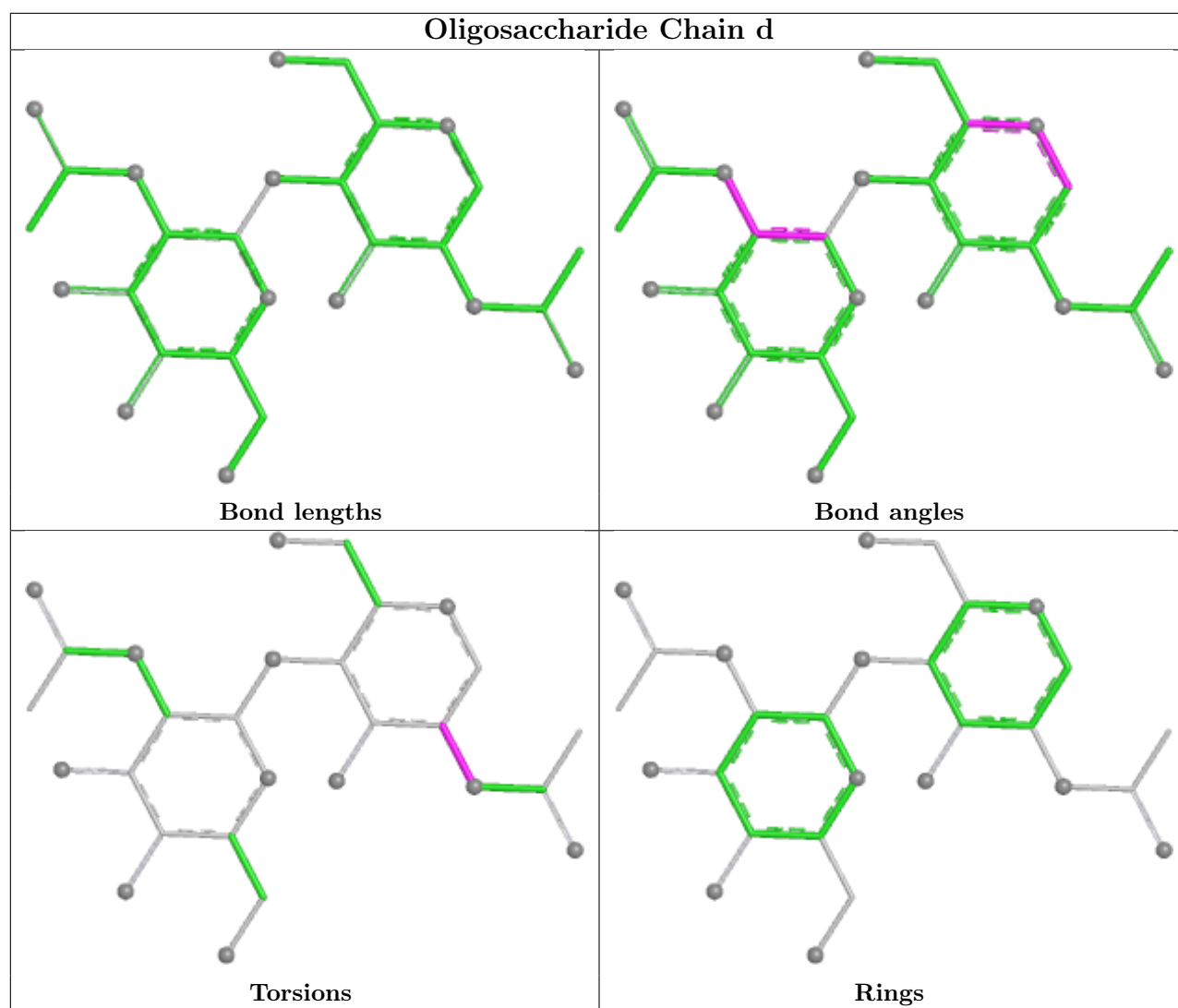


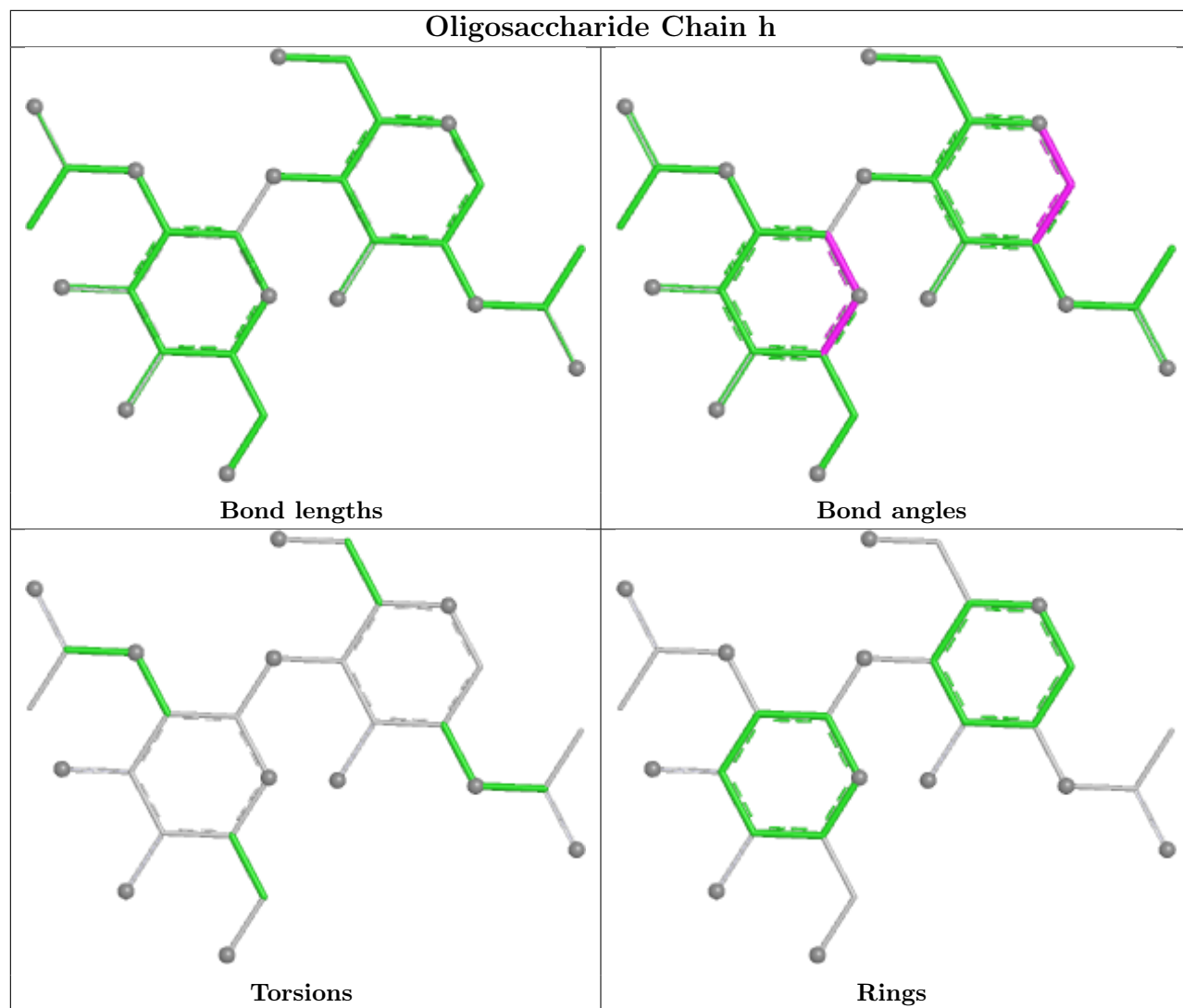


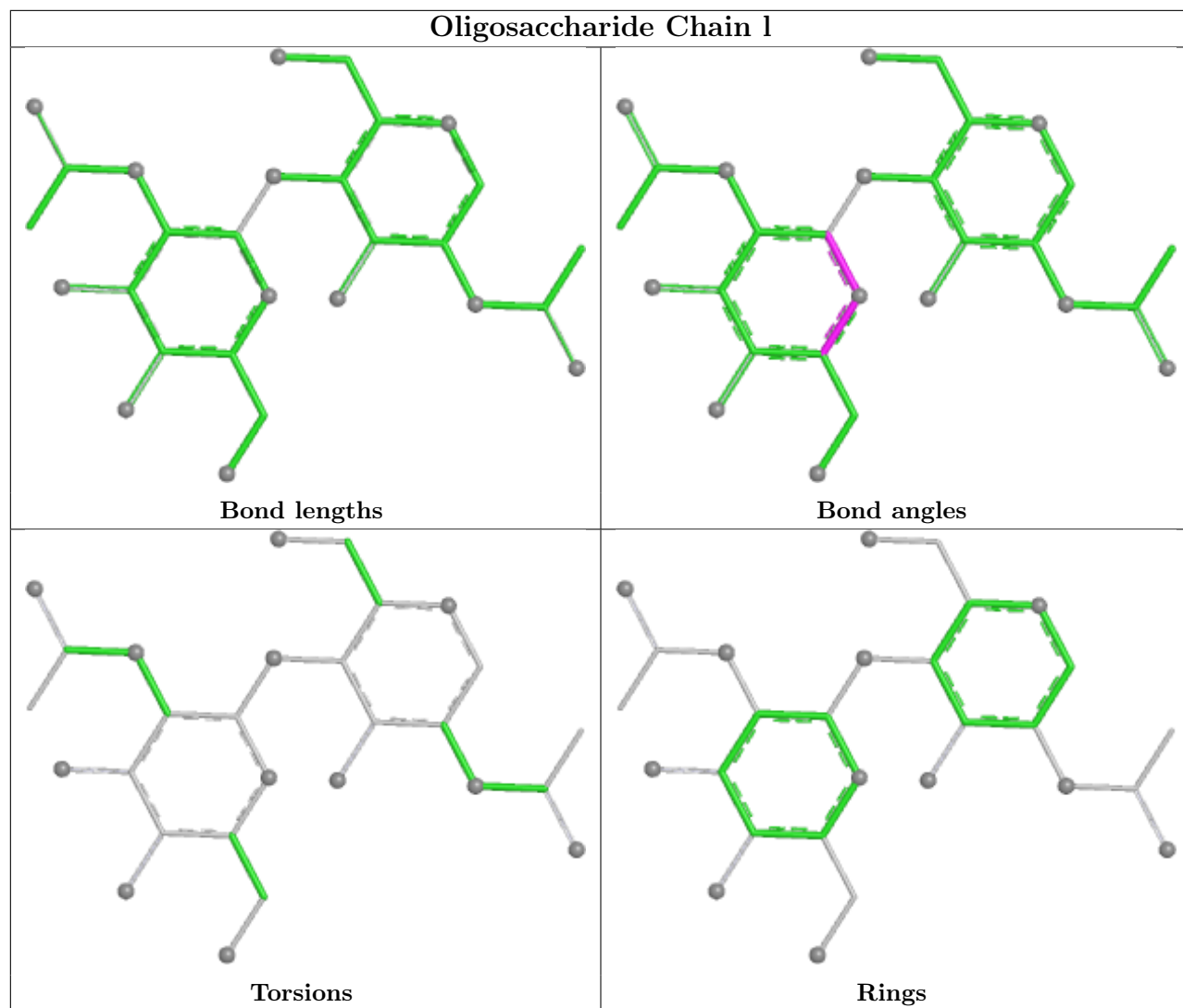


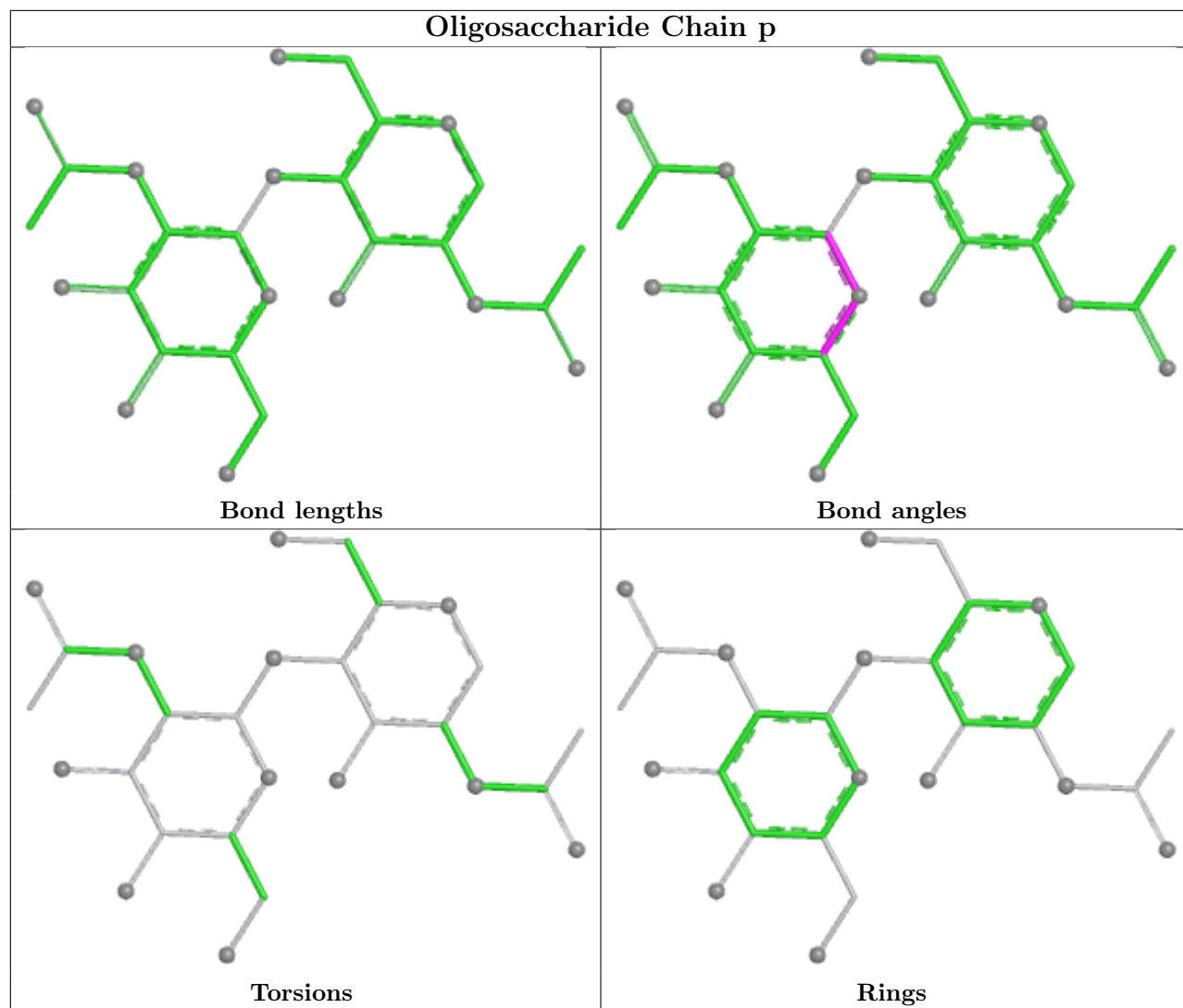


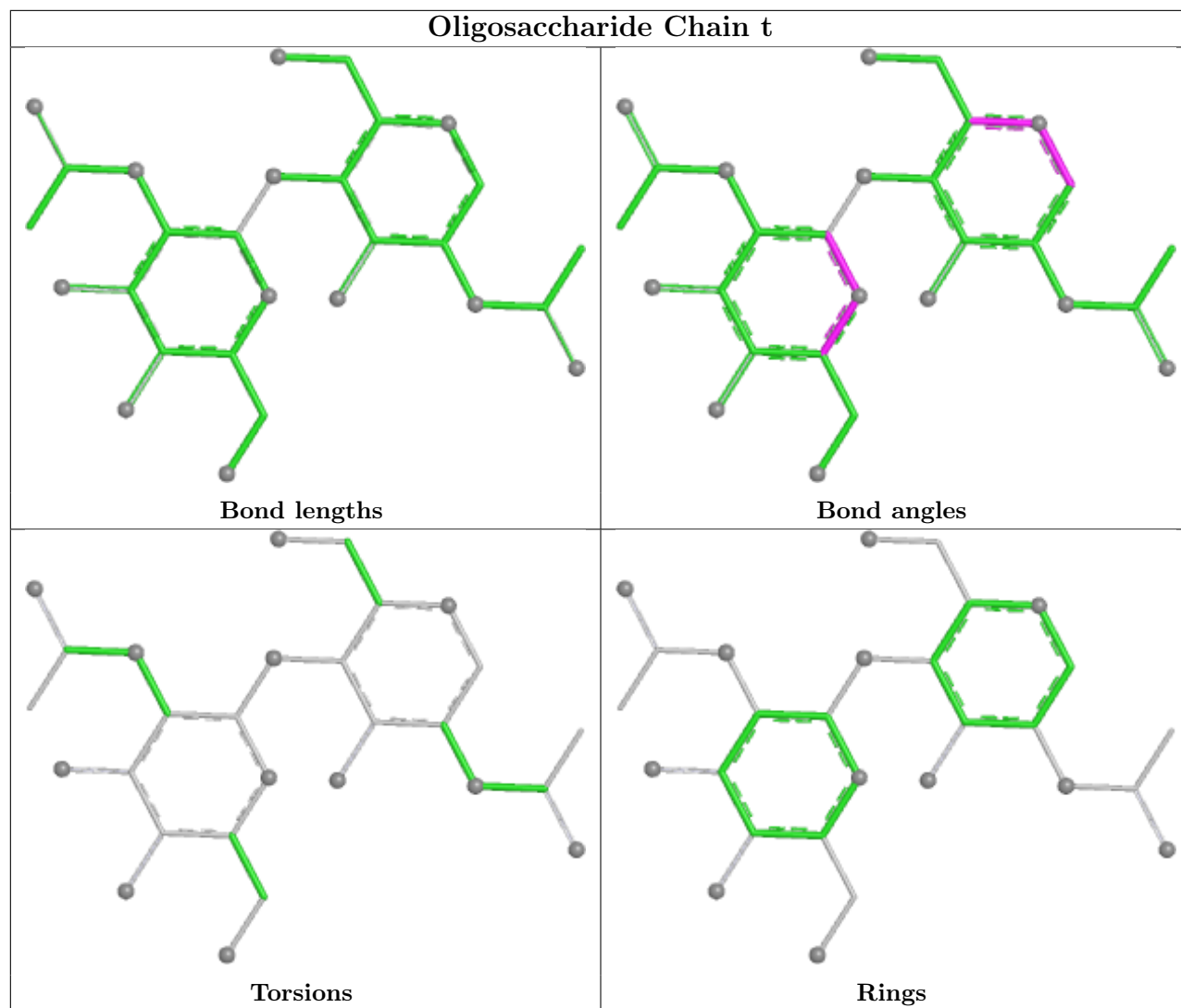


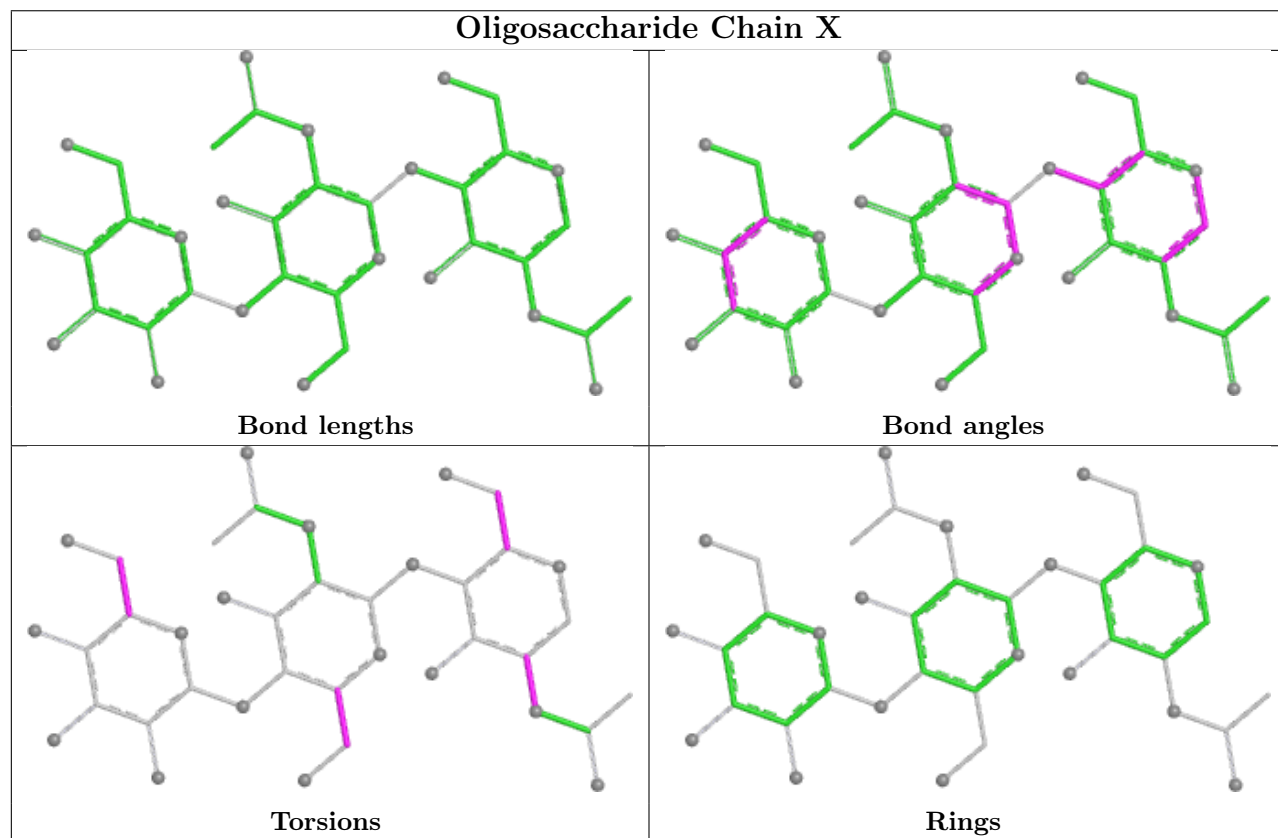
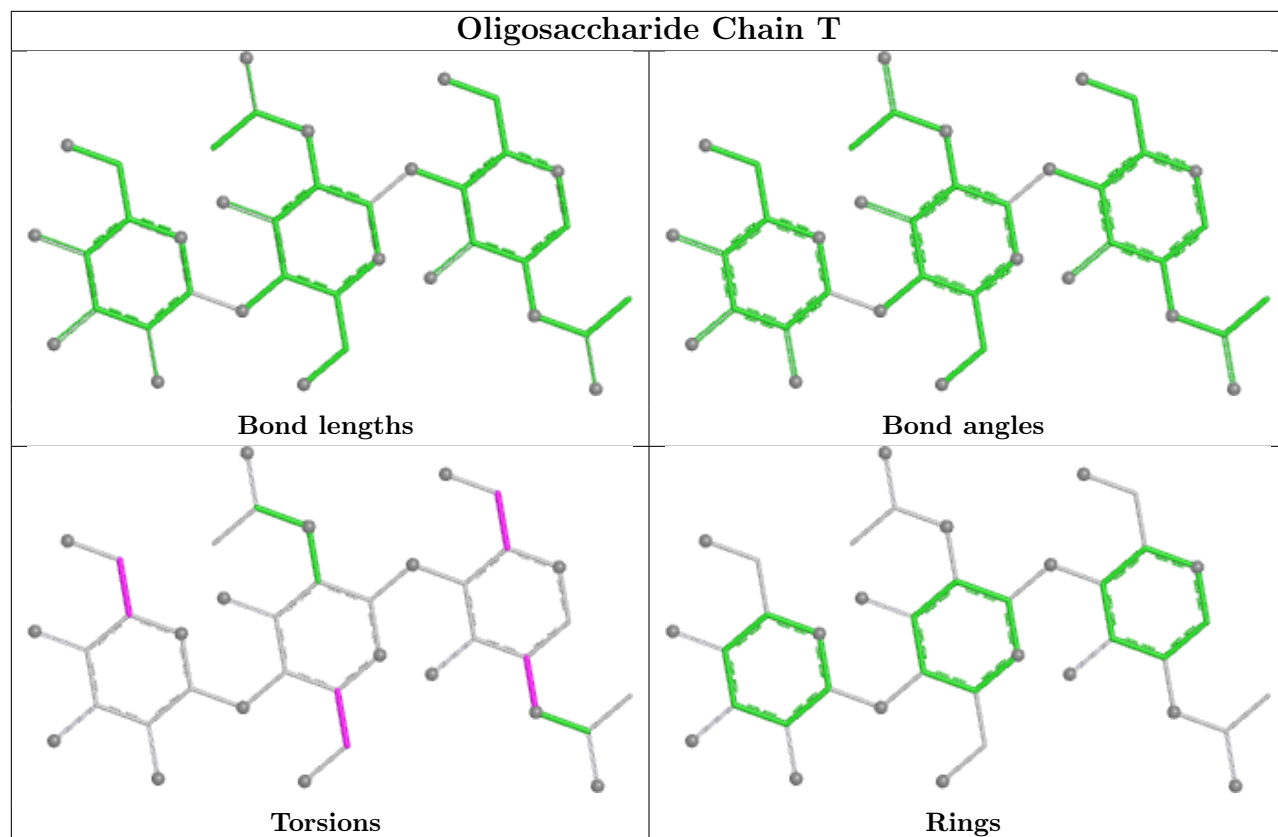


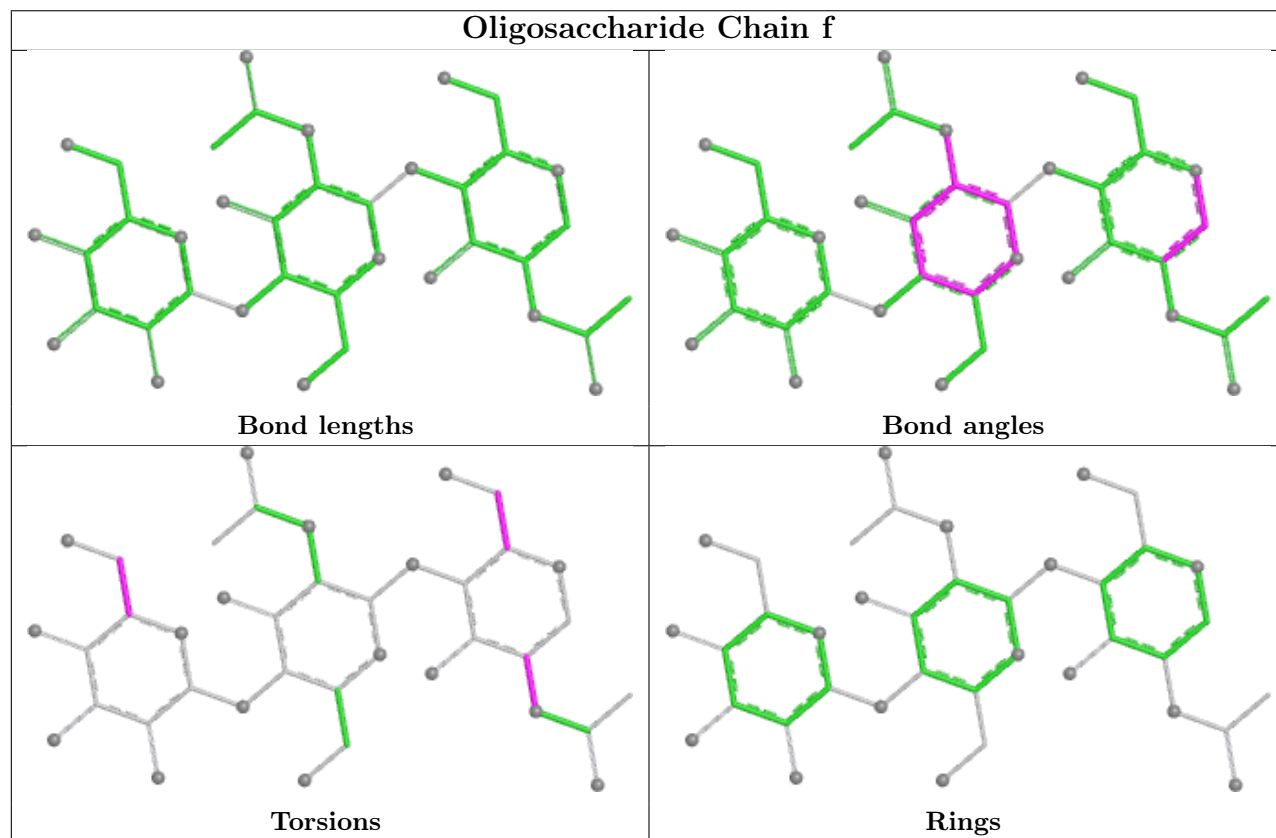
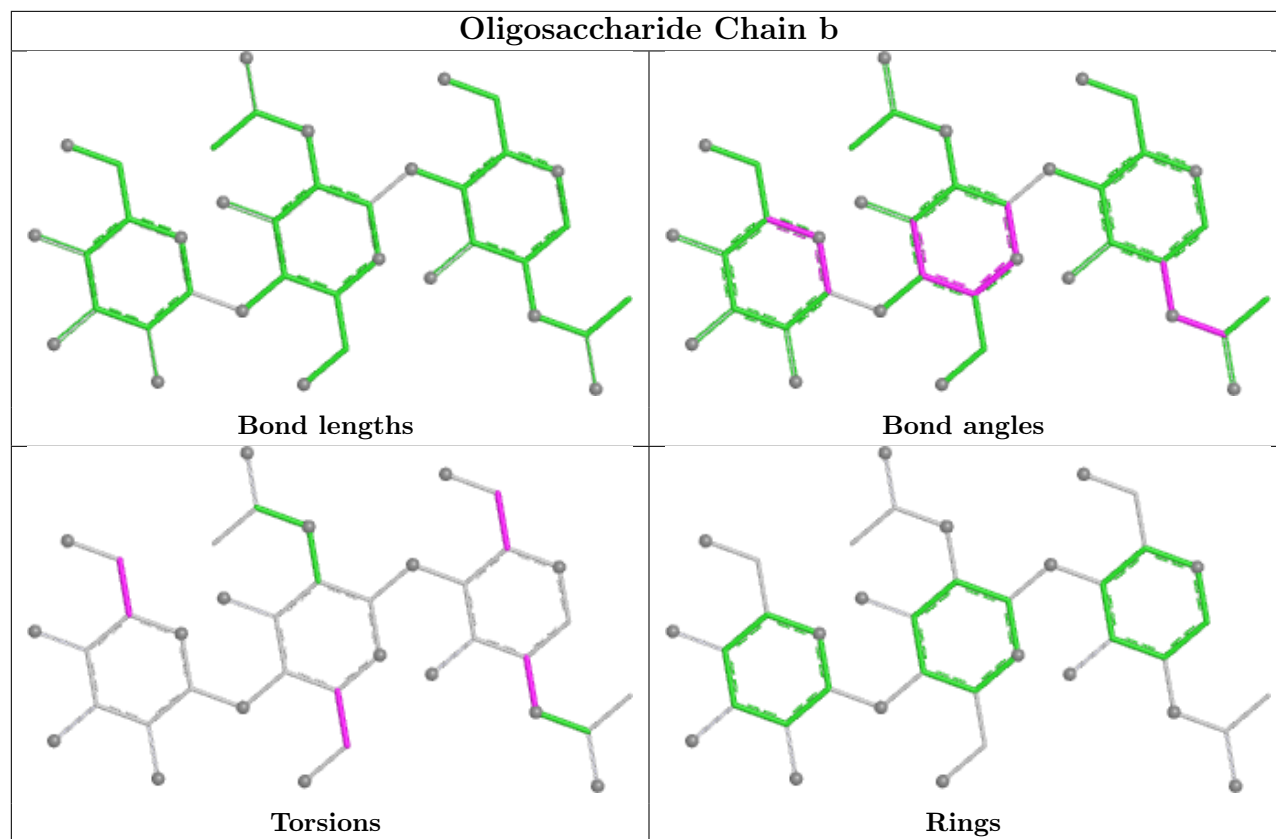


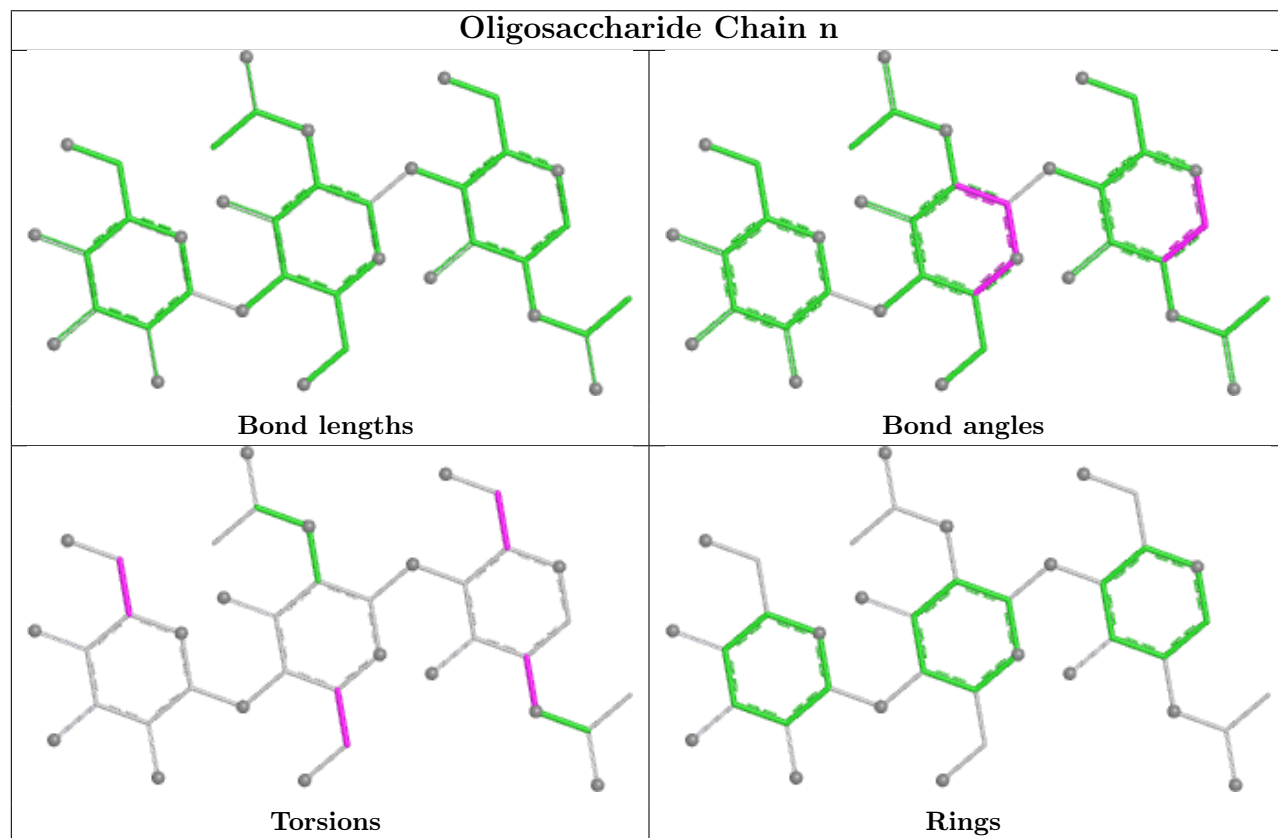
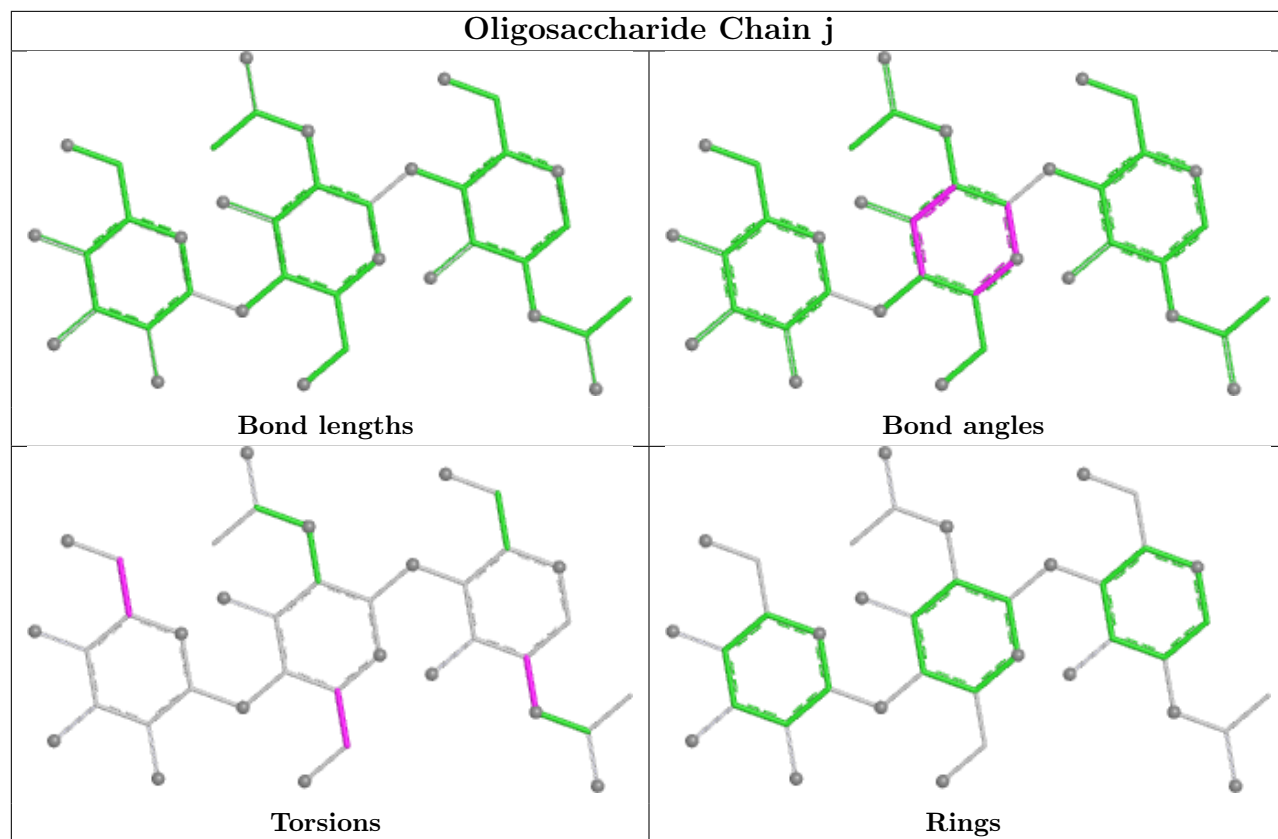


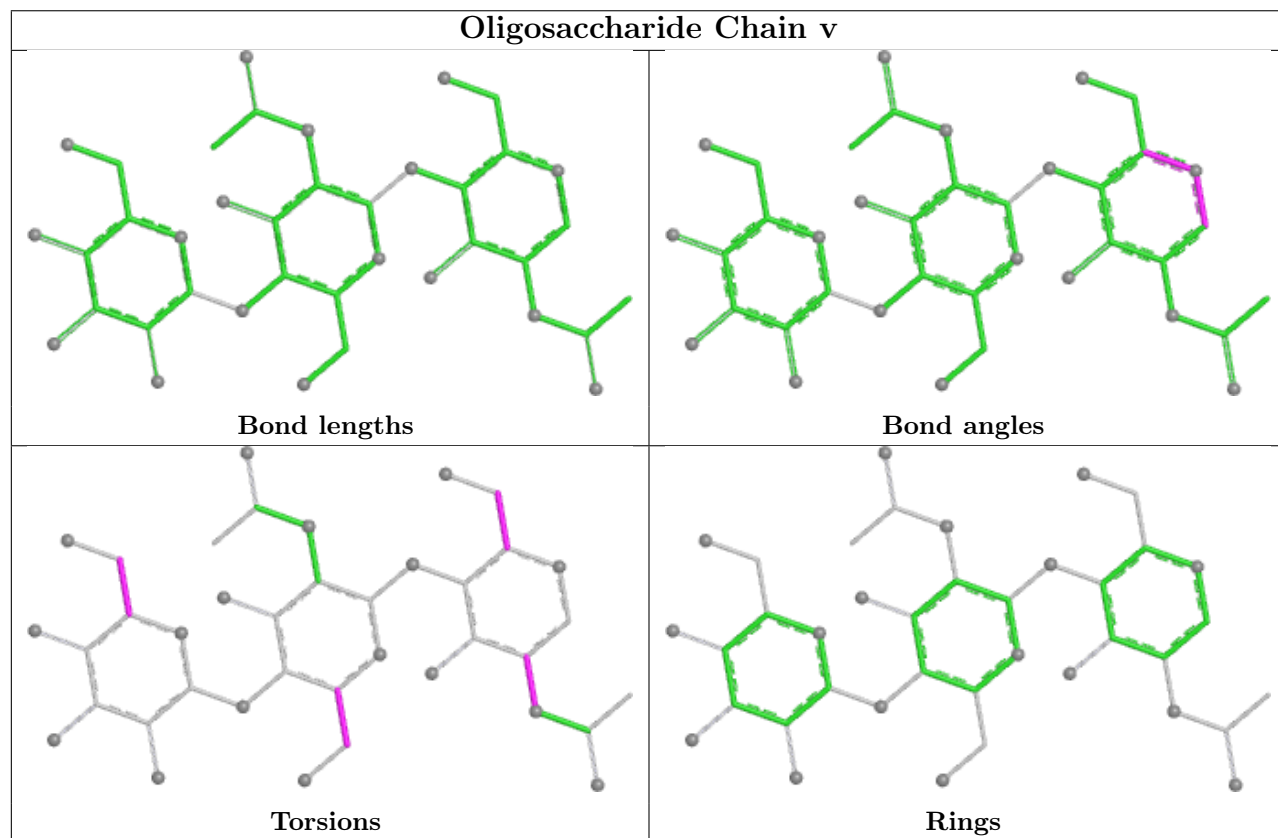
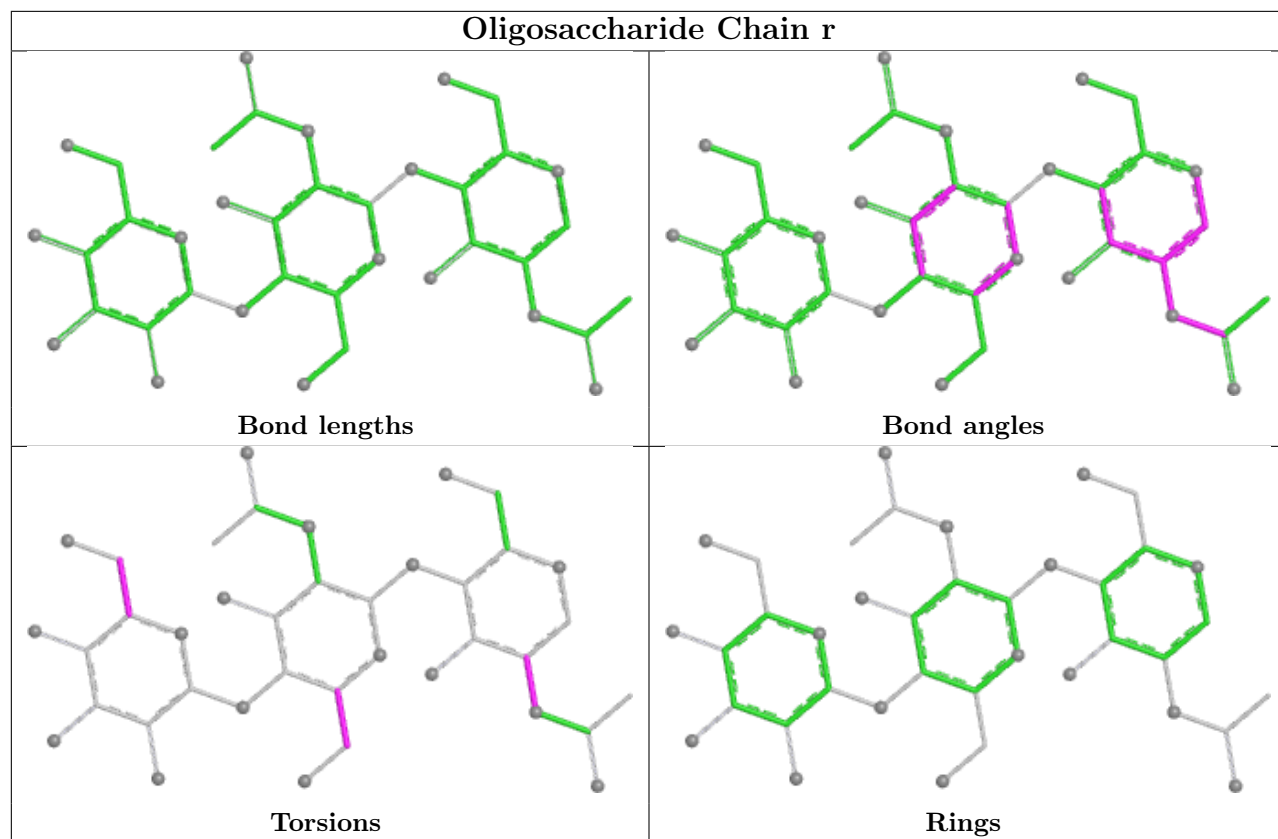












5.6 Ligand geometry

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	501	1	14,14,15	0.42	0	17,19,21	1.02	2 (11%)
6	NAG	F	1002	2	14,14,15	0.38	0	17,19,21	0.89	1 (5%)
6	NAG	O	504	1	14,14,15	0.38	0	17,19,21	1.09	1 (5%)
6	NAG	O	503	1	14,14,15	0.44	0	17,19,21	0.82	1 (5%)
6	NAG	K	502	1	14,14,15	0.36	0	17,19,21	0.89	1 (5%)
6	NAG	N	1003	2	14,14,15	0.58	0	17,19,21	0.95	1 (5%)
6	NAG	A	504	1	14,14,15	0.48	0	17,19,21	0.99	1 (5%)
6	NAG	C	505	1	14,14,15	0.26	0	17,19,21	0.73	0
6	NAG	P	1004	2	14,14,15	0.37	0	17,19,21	0.90	1 (5%)
6	NAG	A	503	1	14,14,15	0.38	0	17,19,21	0.85	0
8	GLC	I	506	-	12,12,12	0.59	0	17,17,17	0.54	0
6	NAG	F	1003	2	14,14,15	0.46	0	17,19,21	0.63	0
6	NAG	K	503	1	14,14,15	0.36	0	17,19,21	1.24	2 (11%)
6	NAG	J	1003	2	14,14,15	0.31	0	17,19,21	0.95	1 (5%)
6	NAG	J	1004	2	14,14,15	0.48	0	17,19,21	0.90	1 (5%)
6	NAG	L	1003	2	14,14,15	0.43	0	17,19,21	1.09	2 (11%)
6	NAG	L	1004	2	14,14,15	0.38	0	17,19,21	0.63	0
6	NAG	M	502	1	14,14,15	0.28	0	17,19,21	0.94	1 (5%)
8	GLC	L	1002	-	12,12,12	0.69	0	17,17,17	0.99	1 (5%)
6	NAG	I	505	1	14,14,15	0.33	0	17,19,21	0.64	0
6	NAG	G	505	1	14,14,15	0.41	0	17,19,21	1.09	2 (11%)
6	NAG	C	504	1	14,14,15	0.38	0	17,19,21	1.12	2 (11%)
6	NAG	E	503	1	14,14,15	0.55	0	17,19,21	0.94	1 (5%)
6	NAG	N	1002	2	14,14,15	0.38	0	17,19,21	0.81	0
6	NAG	P	1003	2	14,14,15	0.41	0	17,19,21	0.91	1 (5%)
6	NAG	G	501	1	14,14,15	0.39	0	17,19,21	1.26	3 (17%)
8	GLC	M	506	-	12,12,12	0.55	0	17,17,17	0.62	0
8	GLC	P	1002	-	12,12,12	0.57	0	17,17,17	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	G	503	1	14,14,15	0.47	0	17,19,21	1.18	1 (5%)
6	NAG	G	504	1	14,14,15	0.32	0	17,19,21	0.79	0
6	NAG	H	1004	2	14,14,15	0.46	0	17,19,21	0.74	0
6	NAG	I	503	1	14,14,15	0.35	0	17,19,21	1.02	1 (5%)
6	NAG	E	501	1	14,14,15	0.57	0	17,19,21	0.93	0
6	NAG	E	502	1	14,14,15	0.28	0	17,19,21	0.62	0
8	GLC	G	506	-	12,12,12	0.61	0	17,17,17	0.78	0
6	NAG	E	504	1	14,14,15	0.31	0	17,19,21	0.87	1 (5%)
6	NAG	A	505	1	14,14,15	0.42	0	17,19,21	1.12	1 (5%)
6	NAG	C	503	1	14,14,15	0.40	0	17,19,21	0.81	1 (5%)
6	NAG	I	504	1	14,14,15	0.28	0	17,19,21	1.10	2 (11%)
6	NAG	O	502	1	14,14,15	0.33	0	17,19,21	0.73	0
6	NAG	A	501	1	14,14,15	0.36	0	17,19,21	0.62	0
8	GLC	E	506	-	12,12,12	0.63	0	17,17,17	0.77	0
6	NAG	D	1003	2	14,14,15	0.35	0	17,19,21	0.92	1 (5%)
8	GLC	B	1002	-	12,12,12	0.64	0	17,17,17	0.81	1 (5%)
6	NAG	H	1003	2	14,14,15	0.29	0	17,19,21	0.87	1 (5%)
6	NAG	A	502	1	14,14,15	0.25	0	17,19,21	0.88	1 (5%)
6	NAG	K	501	1	14,14,15	0.26	0	17,19,21	0.73	0
6	NAG	L	1005	2	14,14,15	0.51	0	17,19,21	1.82	5 (29%)
6	NAG	C	501	1	14,14,15	0.35	0	17,19,21	0.77	1 (5%)
6	NAG	M	505	1	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
6	NAG	D	1002	2	14,14,15	0.33	0	17,19,21	0.91	1 (5%)
6	NAG	M	501	1	14,14,15	0.45	0	17,19,21	1.08	1 (5%)
6	NAG	B	1004	2	14,14,15	0.48	0	17,19,21	0.56	0
8	GLC	C	506	-	12,12,12	0.59	0	17,17,17	0.69	0
6	NAG	H	1002	2	14,14,15	0.38	0	17,19,21	0.71	0
6	NAG	M	503	1	14,14,15	0.37	0	17,19,21	1.02	1 (5%)
6	NAG	M	504	1	14,14,15	0.37	0	17,19,21	1.16	1 (5%)
6	NAG	B	1003	2	14,14,15	0.35	0	17,19,21	0.72	0
6	NAG	O	505	1	14,14,15	0.33	0	17,19,21	0.51	0
6	NAG	I	501	1	14,14,15	0.41	0	17,19,21	0.98	2 (11%)
6	NAG	C	502	1	14,14,15	0.30	0	17,19,21	0.73	1 (5%)
6	NAG	I	502	1	14,14,15	0.34	0	17,19,21	0.56	0
6	NAG	G	502	1	14,14,15	0.26	0	17,19,21	0.61	0
6	NAG	J	1002	2	14,14,15	0.37	0	17,19,21	0.68	0
6	NAG	E	505	1	14,14,15	0.29	0	17,19,21	0.70	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
6	NAG	O	501	1	-	1/6/23/26	0/1/1/1
6	NAG	F	1002	2	-	0/6/23/26	0/1/1/1
6	NAG	O	504	1	-	0/6/23/26	0/1/1/1
6	NAG	O	503	1	-	2/6/23/26	0/1/1/1
6	NAG	K	502	1	-	0/6/23/26	0/1/1/1
6	NAG	N	1003	2	-	2/6/23/26	0/1/1/1
6	NAG	A	504	1	-	1/6/23/26	0/1/1/1
6	NAG	C	505	1	-	2/6/23/26	0/1/1/1
6	NAG	P	1004	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	F	1003	2	-	0/6/23/26	0/1/1/1
6	NAG	K	503	1	-	0/6/23/26	0/1/1/1
6	NAG	J	1003	2	-	1/6/23/26	0/1/1/1
6	NAG	J	1004	2	-	3/6/23/26	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	M	502	1	-	0/6/23/26	0/1/1/1
8	GLC	L	1002	-	-	0/2/22/22	0/1/1/1
6	NAG	I	505	1	-	2/6/23/26	0/1/1/1
6	NAG	G	505	1	-	0/6/23/26	0/1/1/1
6	NAG	C	504	1	-	2/6/23/26	0/1/1/1
6	NAG	E	503	1	-	0/6/23/26	0/1/1/1
6	NAG	N	1002	2	-	0/6/23/26	0/1/1/1
6	NAG	P	1003	2	-	0/6/23/26	0/1/1/1
6	NAG	G	501	1	-	2/6/23/26	0/1/1/1
8	GLC	M	506	-	-	1/2/22/22	0/1/1/1
8	GLC	P	1002	-	-	0/2/22/22	0/1/1/1
6	NAG	G	503	1	-	2/6/23/26	0/1/1/1
6	NAG	G	504	1	-	0/6/23/26	0/1/1/1
6	NAG	H	1004	2	-	1/6/23/26	0/1/1/1
6	NAG	I	503	1	-	0/6/23/26	0/1/1/1
6	NAG	E	501	1	-	2/6/23/26	0/1/1/1
6	NAG	E	502	1	-	0/6/23/26	0/1/1/1
8	GLC	G	506	-	-	0/2/22/22	0/1/1/1
6	NAG	E	504	1	-	0/6/23/26	0/1/1/1
6	NAG	A	505	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	503	1	-	2/6/23/26	0/1/1/1
6	NAG	I	504	1	-	0/6/23/26	0/1/1/1
6	NAG	O	502	1	-	2/6/23/26	0/1/1/1
6	NAG	A	501	1	-	0/6/23/26	0/1/1/1
8	GLC	E	506	-	-	2/2/22/22	0/1/1/1
6	NAG	D	1003	2	-	0/6/23/26	0/1/1/1
8	GLC	B	1002	-	-	0/2/22/22	0/1/1/1
6	NAG	H	1003	2	-	2/6/23/26	0/1/1/1
6	NAG	A	502	1	-	0/6/23/26	0/1/1/1
6	NAG	K	501	1	-	0/6/23/26	0/1/1/1
6	NAG	L	1005	2	-	0/6/23/26	0/1/1/1
6	NAG	C	501	1	-	2/6/23/26	0/1/1/1
6	NAG	M	505	1	-	1/6/23/26	0/1/1/1
6	NAG	D	1002	2	-	0/6/23/26	0/1/1/1
6	NAG	M	501	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1004	2	-	0/6/23/26	0/1/1/1
8	GLC	C	506	-	-	0/2/22/22	0/1/1/1
6	NAG	H	1002	2	-	0/6/23/26	0/1/1/1
6	NAG	M	503	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	O	505	1	-	1/6/23/26	0/1/1/1
6	NAG	I	501	1	-	4/6/23/26	0/1/1/1
6	NAG	C	502	1	-	0/6/23/26	0/1/1/1
6	NAG	I	502	1	-	0/6/23/26	0/1/1/1
6	NAG	G	502	1	-	0/6/23/26	0/1/1/1
6	NAG	J	1002	2	-	0/6/23/26	0/1/1/1
6	NAG	E	505	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1005	NAG	C1-O5-C5	5.27	119.25	112.19
6	G	503	NAG	C1-O5-C5	4.15	117.75	112.19
6	O	504	NAG	C1-O5-C5	3.90	117.41	112.19
6	K	503	NAG	C1-O5-C5	3.39	116.72	112.19
6	I	504	NAG	C1-O5-C5	3.33	116.64	112.19
6	A	505	NAG	C1-O5-C5	3.21	116.48	112.19
6	C	504	NAG	C1-O5-C5	3.09	116.32	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1003	NAG	C1-O5-C5	3.05	116.27	112.19
6	K	503	NAG	C4-C3-C2	-3.04	106.56	111.02
6	L	1005	NAG	O5-C1-C2	-2.87	106.85	111.29
6	L	1003	NAG	C4-C3-C2	2.86	115.21	111.02
6	M	502	NAG	C1-O5-C5	2.83	115.97	112.19
6	G	501	NAG	O5-C1-C2	-2.76	107.02	111.29
6	A	502	NAG	O5-C1-C2	-2.76	107.03	111.29
6	C	503	NAG	C1-O5-C5	2.72	115.83	112.19
6	A	504	NAG	C1-O5-C5	2.63	115.71	112.19
8	L	1002	GLC	C1-C2-C3	2.59	115.64	110.36
6	P	1003	NAG	C4-C3-C2	2.47	114.64	111.02
6	M	503	NAG	C3-C4-C5	2.46	114.69	110.23
6	G	501	NAG	C3-C4-C5	2.45	114.68	110.23
6	E	504	NAG	C1-O5-C5	2.44	115.45	112.19
6	O	501	NAG	C1-C2-N2	2.40	114.22	110.43
6	F	1002	NAG	C4-C3-C2	2.38	114.51	111.02
6	J	1004	NAG	C1-O5-C5	2.36	115.35	112.19
6	P	1004	NAG	C1-C2-N2	-2.34	106.74	110.43
6	C	501	NAG	O5-C1-C2	-2.28	107.76	111.29
6	D	1002	NAG	C4-C3-C2	2.28	114.36	111.02
6	M	504	NAG	C4-C3-C2	2.24	114.31	111.02
6	G	505	NAG	C1-O5-C5	2.19	115.12	112.19
6	M	501	NAG	O5-C1-C2	-2.19	107.90	111.29
6	C	502	NAG	C1-O5-C5	2.19	115.12	112.19
6	L	1003	NAG	C2-N2-C7	2.18	125.83	122.90
6	I	503	NAG	C3-C4-C5	2.18	114.19	110.23
6	G	505	NAG	O5-C1-C2	-2.15	107.96	111.29
8	B	1002	GLC	C1-C2-C3	2.13	114.70	110.36
6	N	1003	NAG	C1-C2-N2	-2.11	107.10	110.43
6	I	504	NAG	C4-C3-C2	-2.11	107.93	111.02
6	L	1005	NAG	O5-C5-C4	2.08	115.90	110.83
6	L	1005	NAG	C3-C4-C5	2.08	114.00	110.23
6	G	501	NAG	C1-C2-N2	2.07	113.70	110.43
6	C	504	NAG	C4-C3-C2	-2.06	108.00	111.02
6	J	1003	NAG	O5-C5-C6	2.06	111.66	107.66
6	L	1005	NAG	C4-C3-C2	-2.05	108.01	111.02
6	D	1003	NAG	C4-C3-C2	2.05	114.02	111.02
6	I	501	NAG	O5-C1-C2	-2.04	108.13	111.29
6	I	501	NAG	C2-N2-C7	2.04	125.63	122.90
6	E	503	NAG	C4-C3-C2	2.04	114.00	111.02
6	O	501	NAG	C2-N2-C7	2.03	125.62	122.90
6	O	503	NAG	C1-O5-C5	2.03	114.91	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	502	NAG	C1-O5-C5	2.02	114.89	112.19
6	M	505	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	501	NAG	C1-C2-N2-C7
6	O	501	NAG	C1-C2-N2-C7
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
6	O	503	NAG	C4-C5-C6-O6
6	J	1004	NAG	C4-C5-C6-O6
6	C	501	NAG	C4-C5-C6-O6
6	G	503	NAG	C4-C5-C6-O6
6	I	501	NAG	C4-C5-C6-O6
8	I	506	GLC	C4-C5-C6-O6
6	J	1004	NAG	O5-C5-C6-O6
6	O	502	NAG	O5-C5-C6-O6
6	I	501	NAG	O5-C5-C6-O6
6	O	502	NAG	C4-C5-C6-O6
6	N	1003	NAG	C4-C5-C6-O6
6	C	505	NAG	C4-C5-C6-O6
8	E	506	GLC	C4-C5-C6-O6
8	I	506	GLC	O5-C5-C6-O6
6	I	505	NAG	C4-C5-C6-O6
6	M	501	NAG	C4-C5-C6-O6
6	N	1003	NAG	O5-C5-C6-O6
8	M	506	GLC	C4-C5-C6-O6
6	I	501	NAG	C1-C2-N2-C7
6	M	501	NAG	C1-C2-N2-C7
8	E	506	GLC	O5-C5-C6-O6
6	H	1003	NAG	C4-C5-C6-O6
6	C	505	NAG	O5-C5-C6-O6
6	C	504	NAG	C4-C5-C6-O6
6	E	501	NAG	C3-C2-N2-C7
6	M	501	NAG	C3-C2-N2-C7
6	C	504	NAG	O5-C5-C6-O6
6	A	503	NAG	O5-C5-C6-O6

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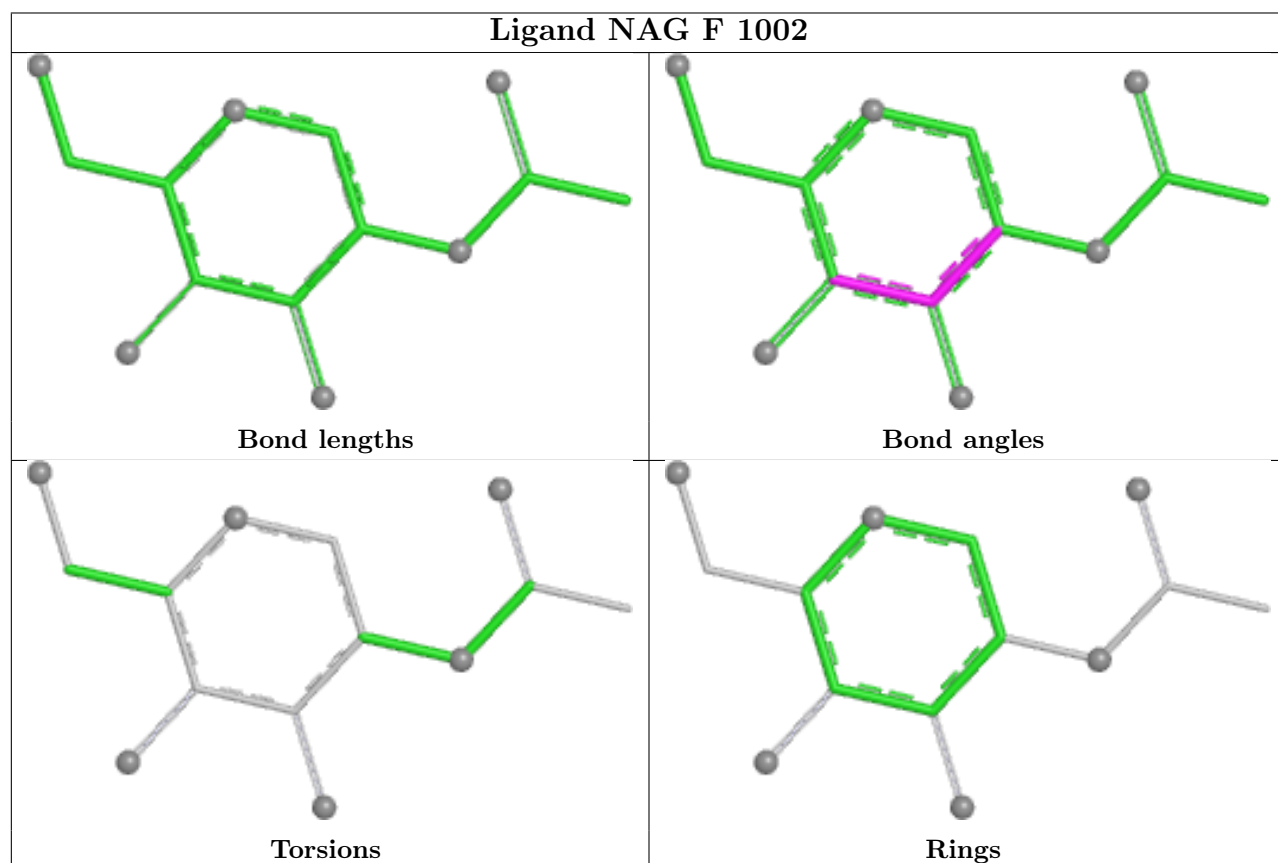
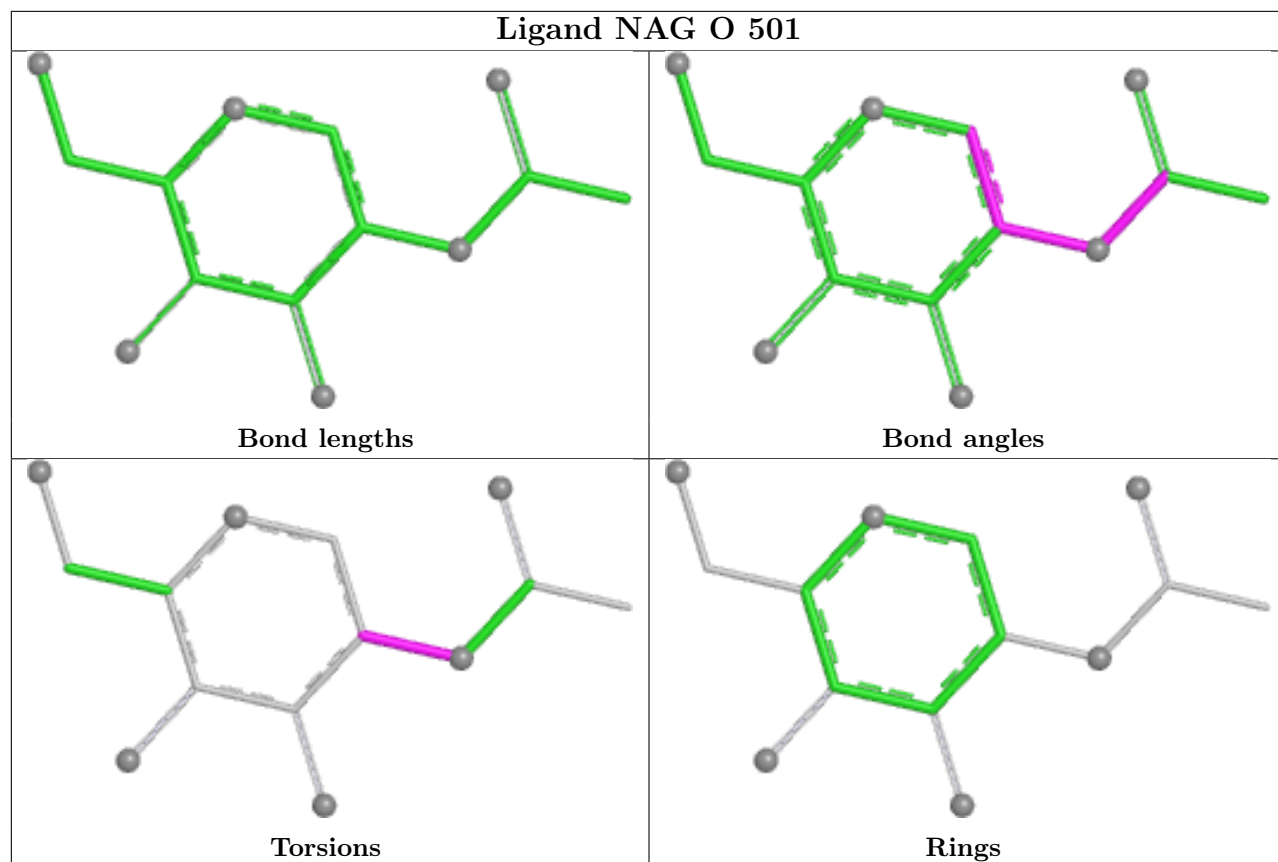
Mol	Chain	Res	Type	Atoms
6	M	505	NAG	O5-C5-C6-O6
6	A	504	NAG	C1-C2-N2-C7
6	E	501	NAG	C1-C2-N2-C7
6	H	1004	NAG	C1-C2-N2-C7
6	J	1003	NAG	C1-C2-N2-C7
6	J	1004	NAG	C1-C2-N2-C7
6	G	501	NAG	C3-C2-N2-C7
6	I	501	NAG	C3-C2-N2-C7
6	I	505	NAG	O5-C5-C6-O6
6	H	1003	NAG	O5-C5-C6-O6
6	O	505	NAG	C4-C5-C6-O6

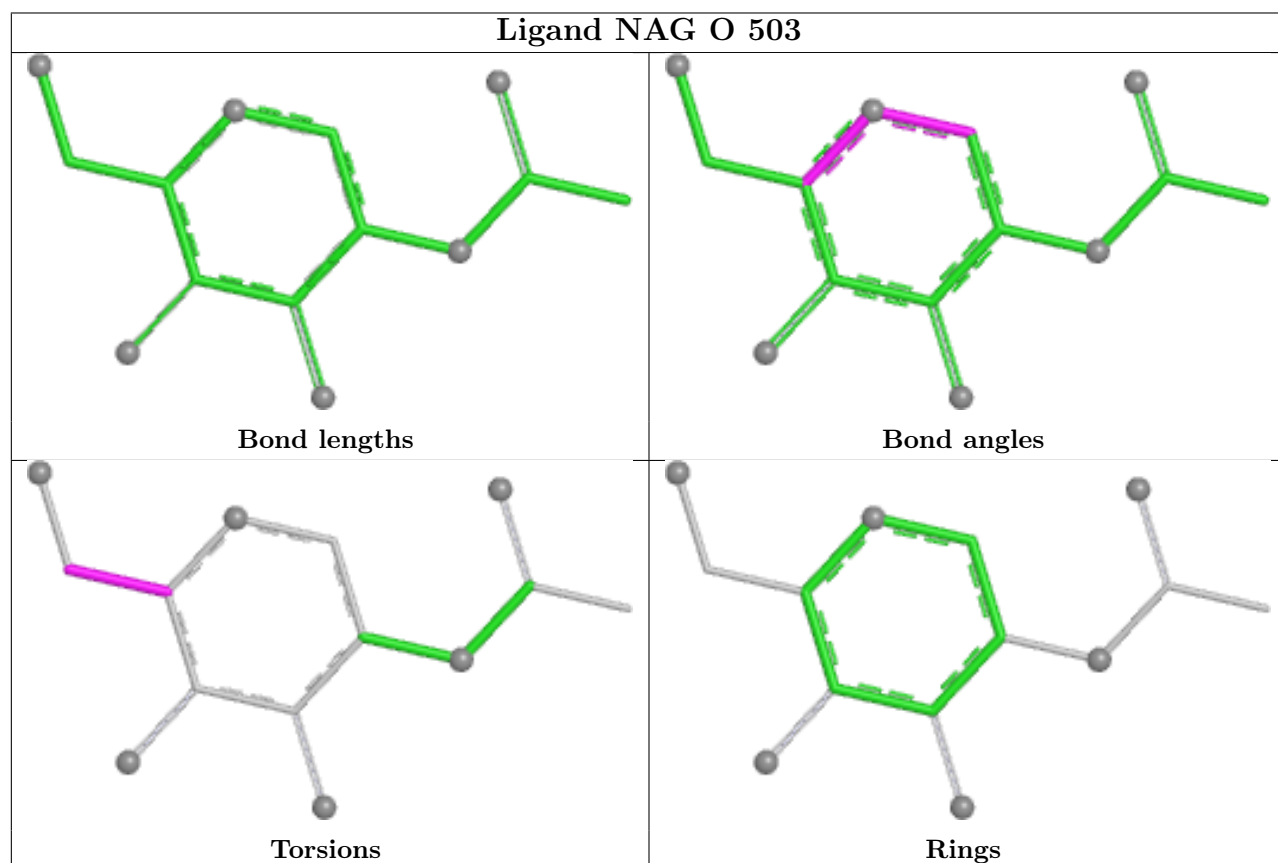
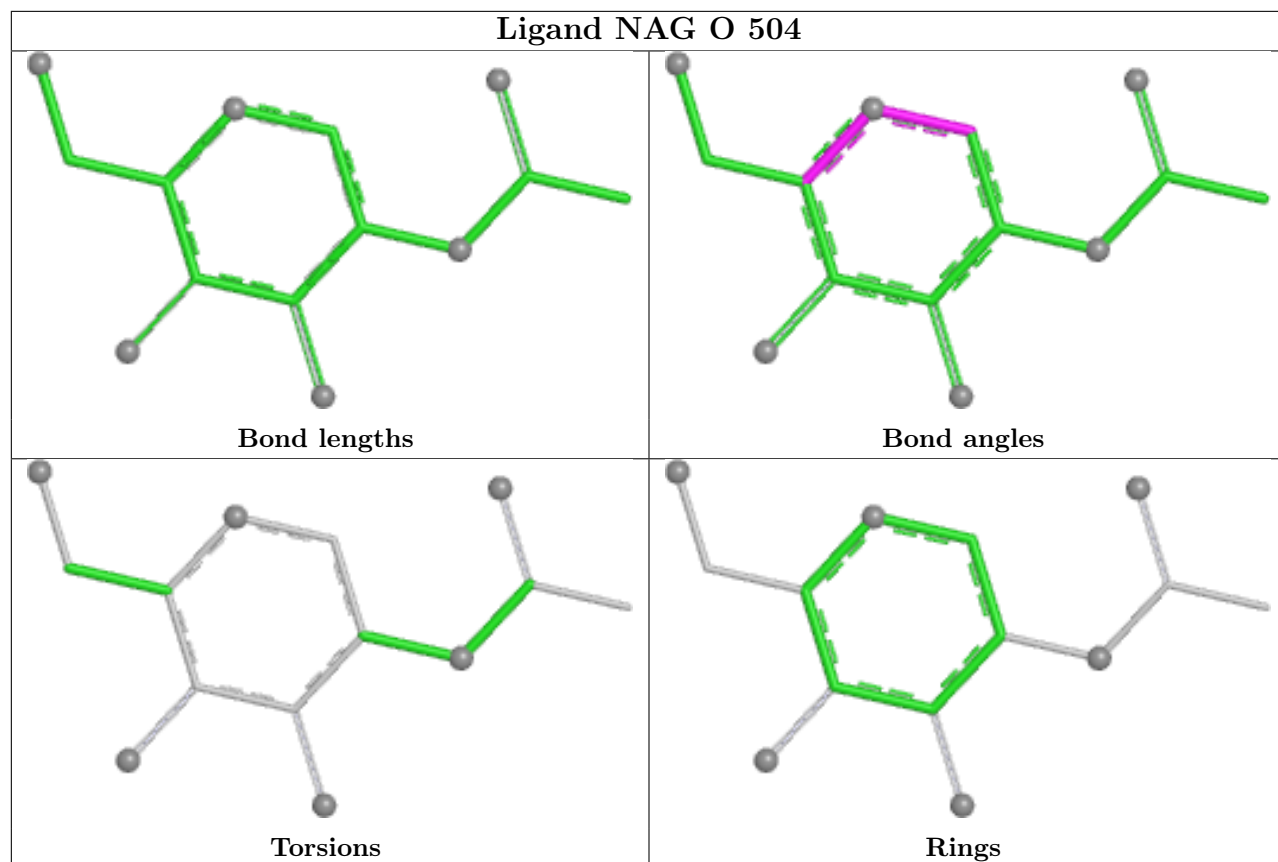
There are no ring outliers.

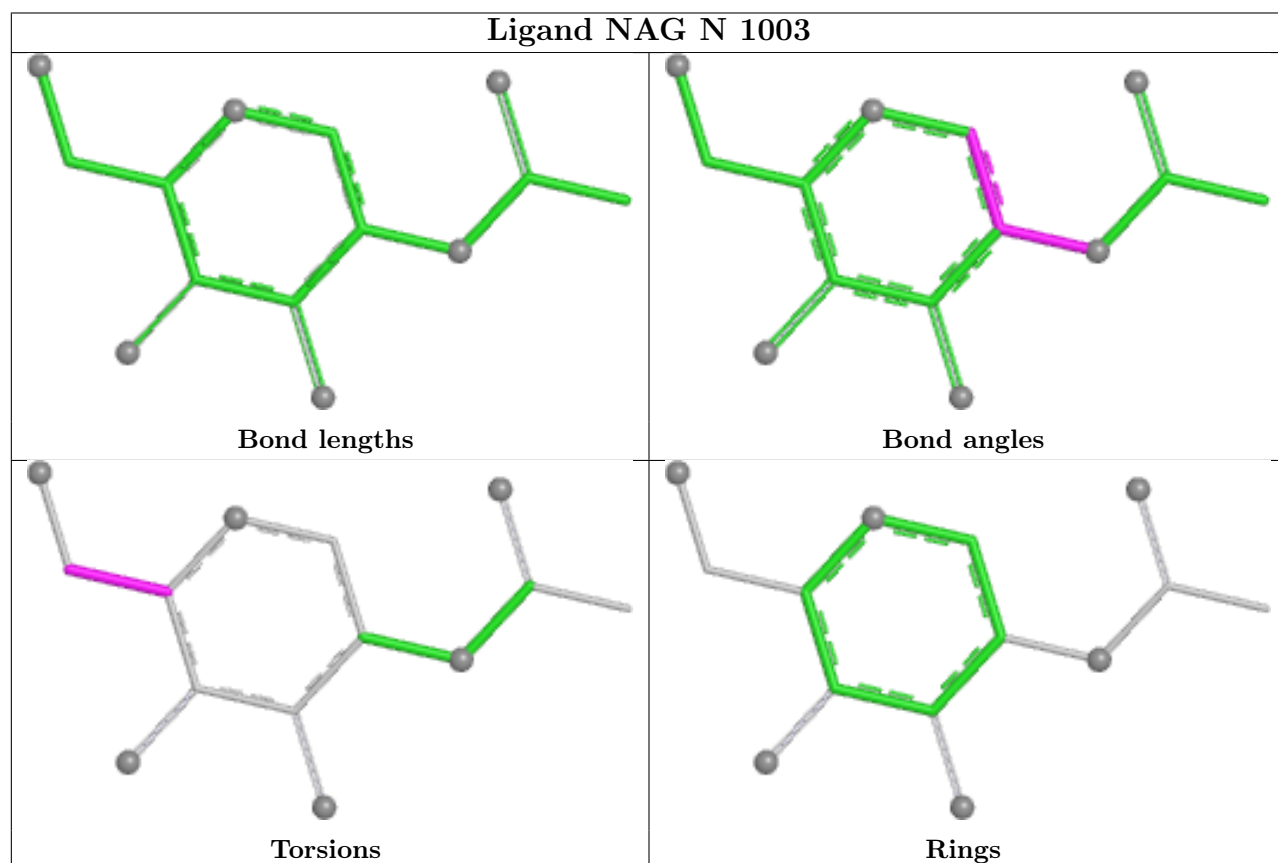
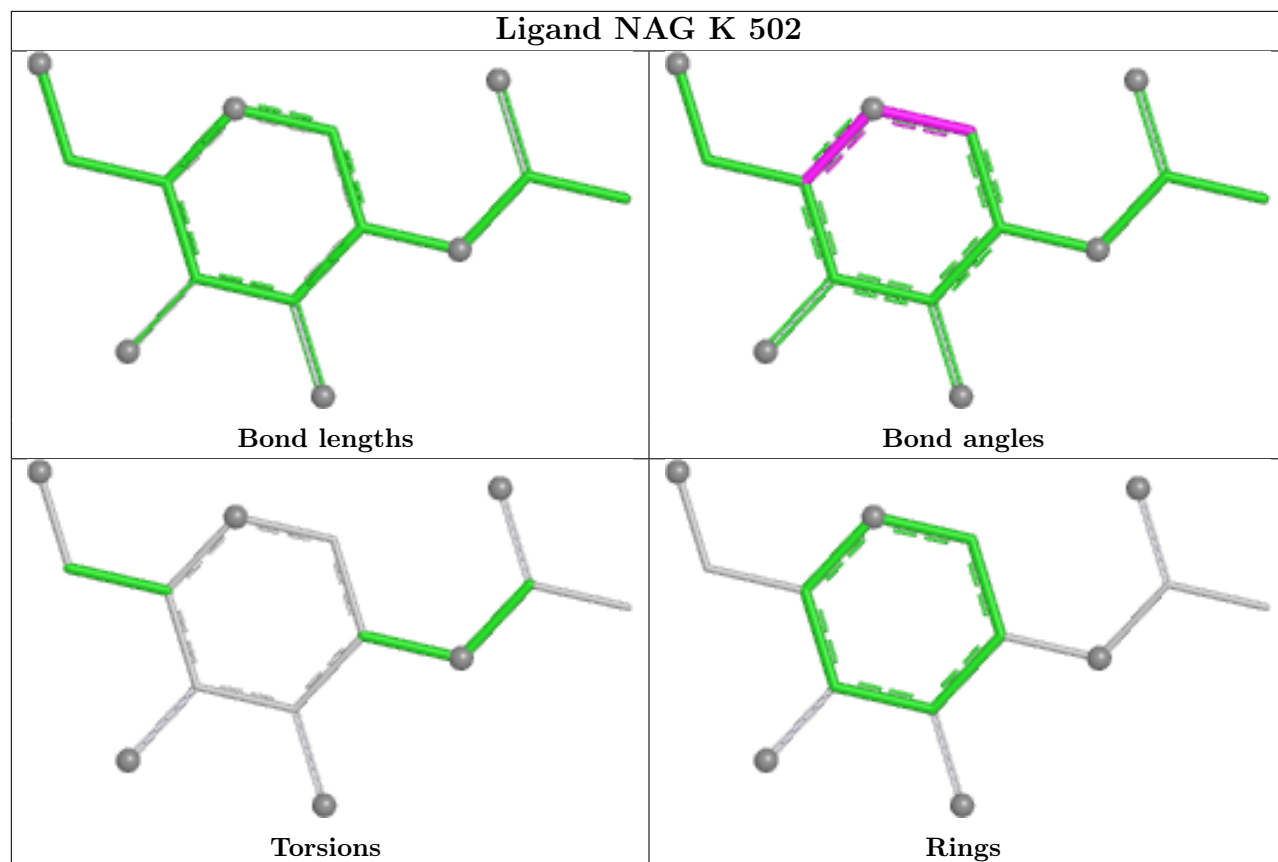
1 monomer is involved in 1 short contact:

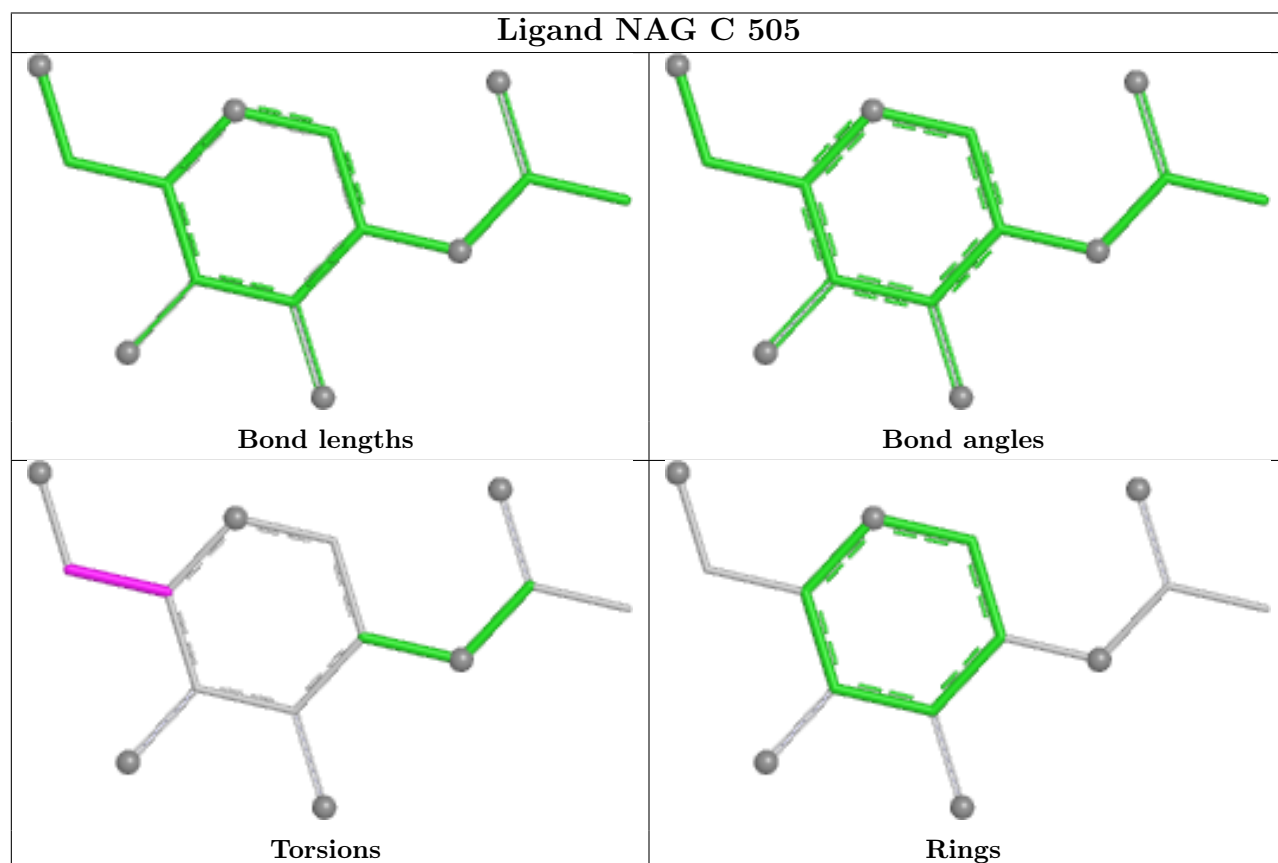
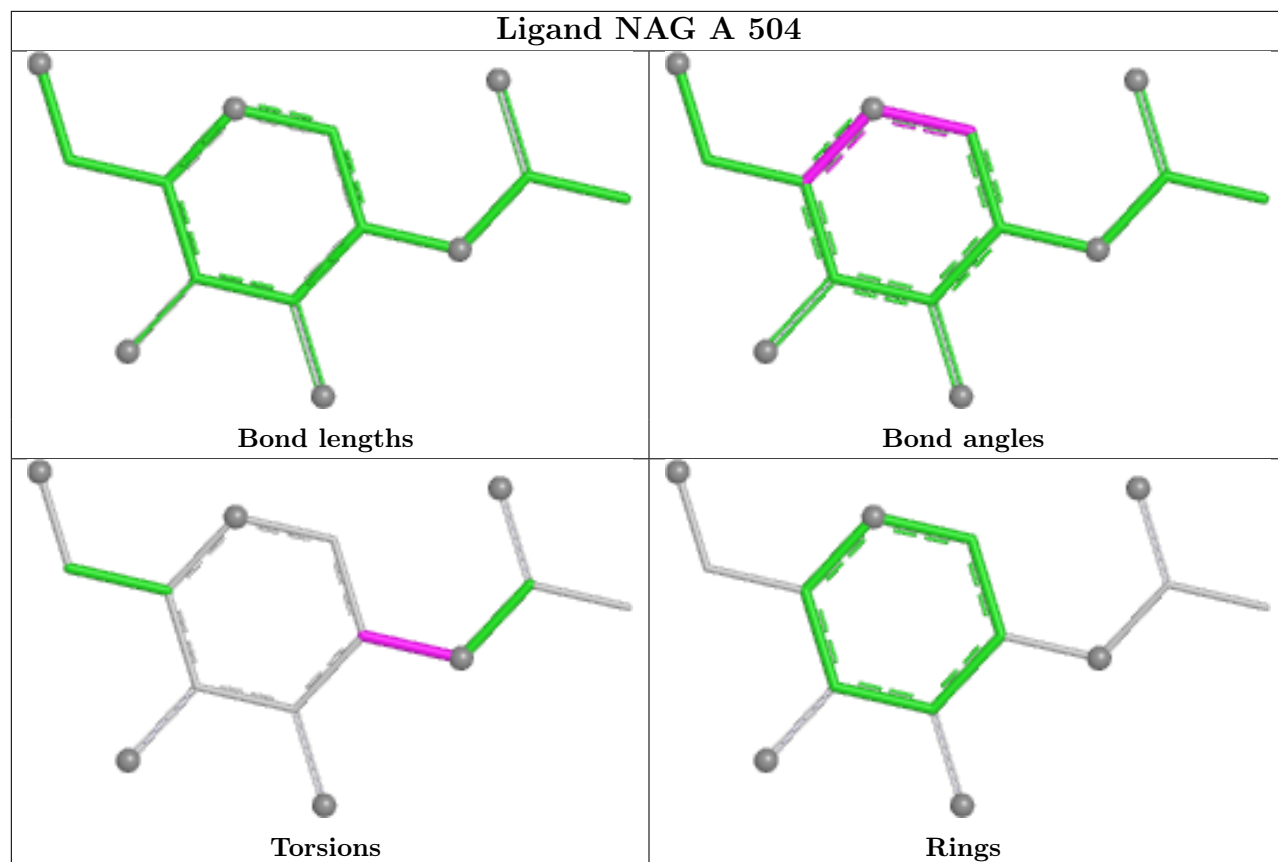
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	504	NAG	1	0

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.

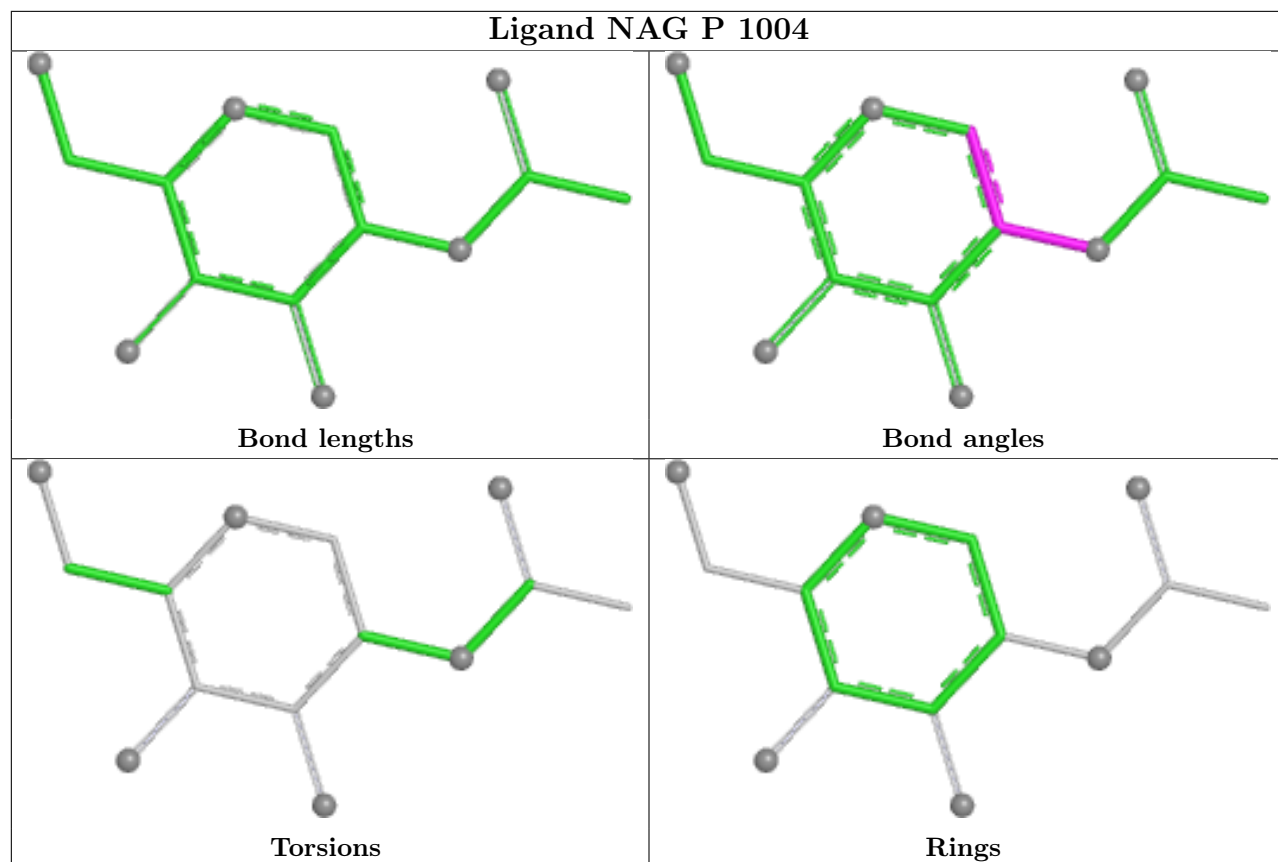




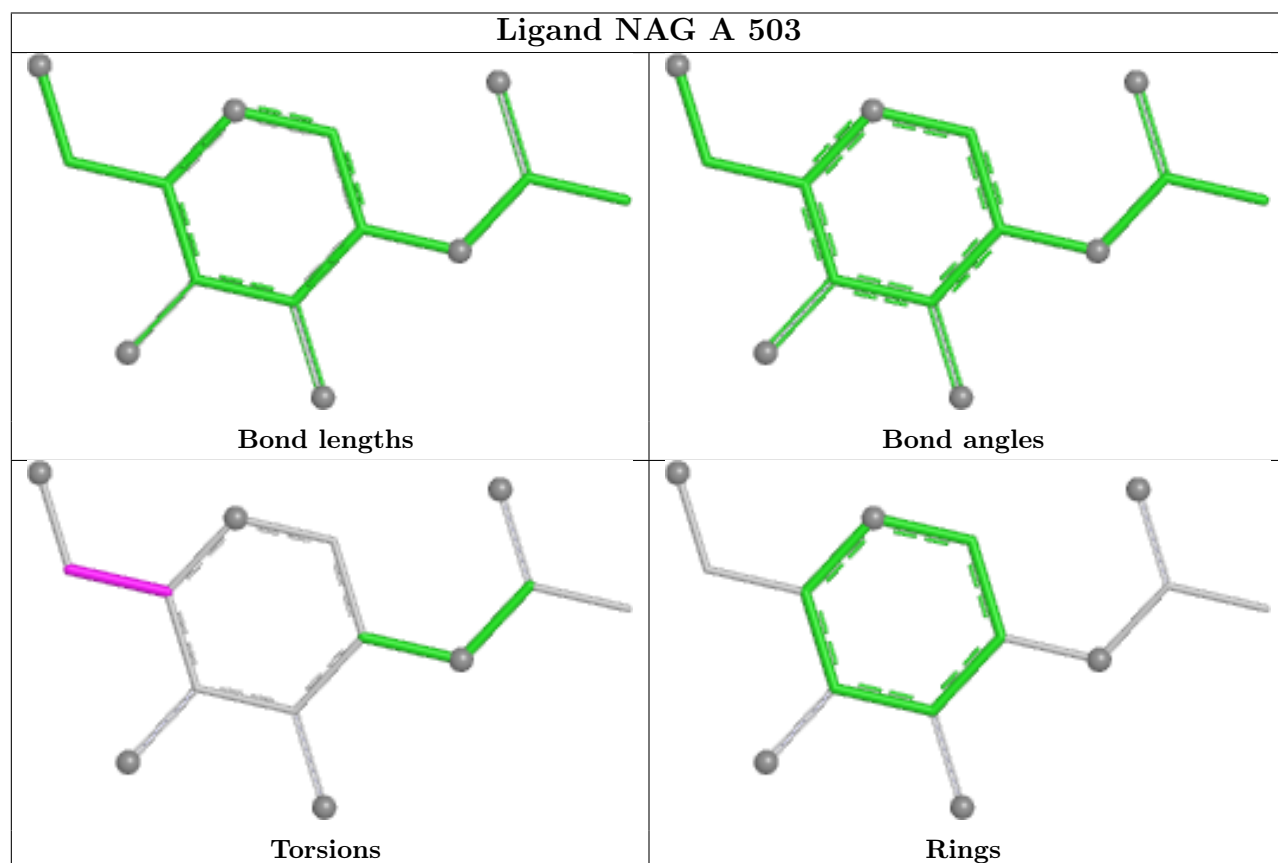




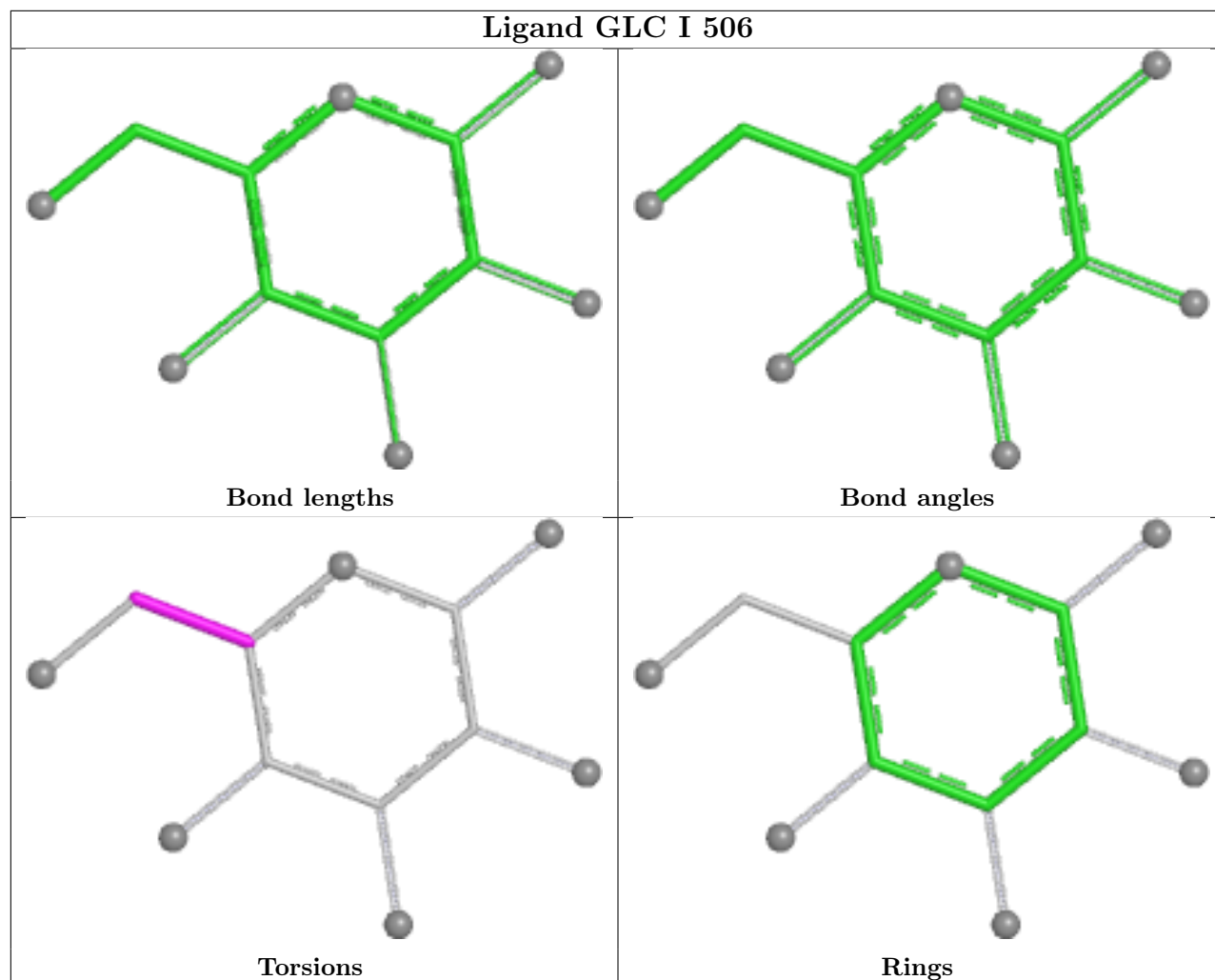
Ligand NAG P 1004



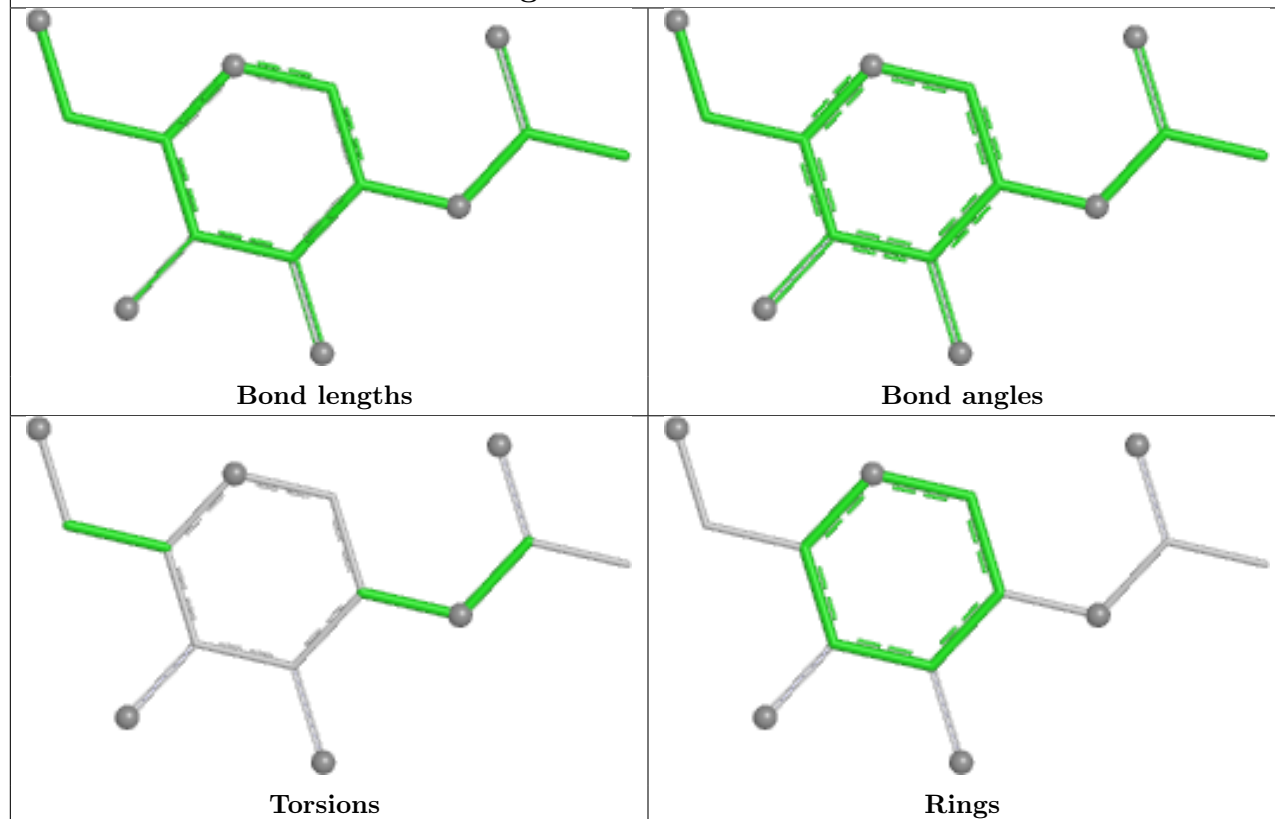
Ligand NAG A 503



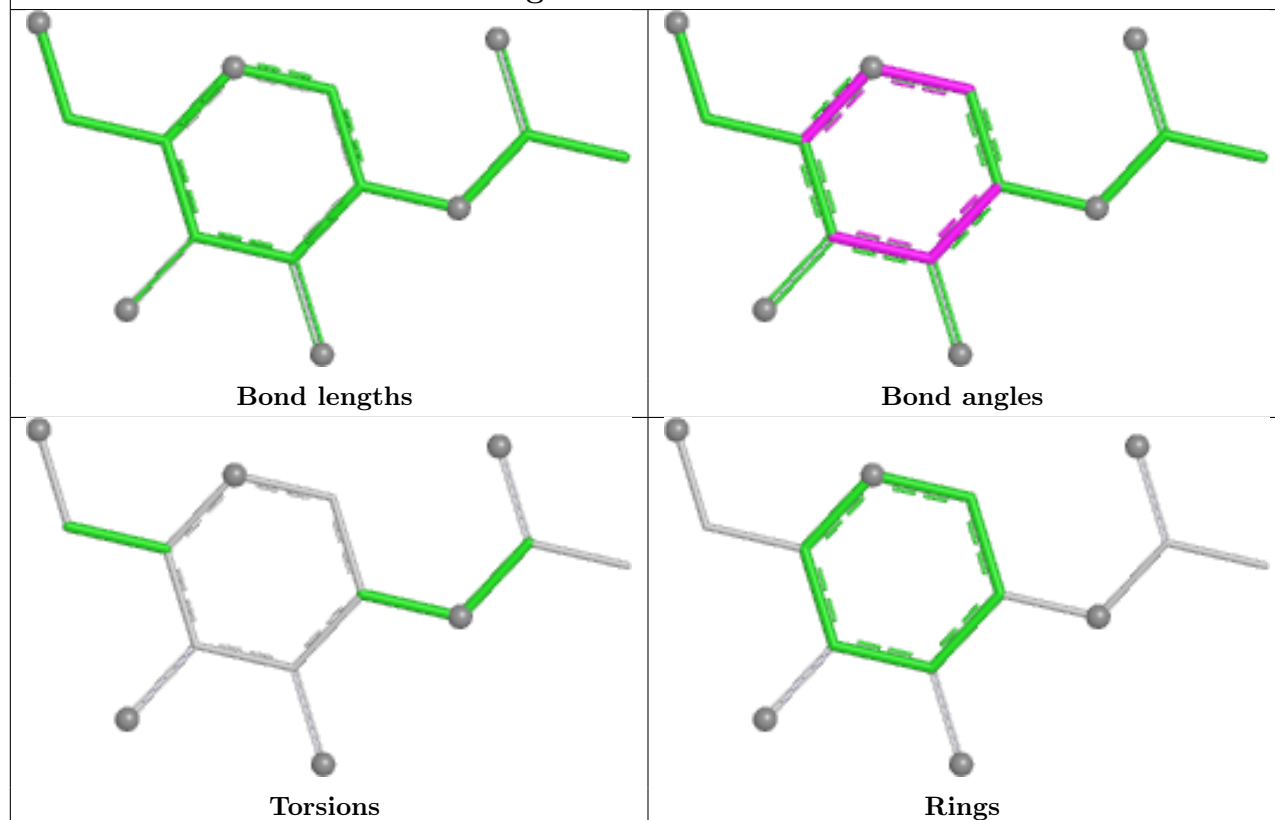
Ligand GLC I 506



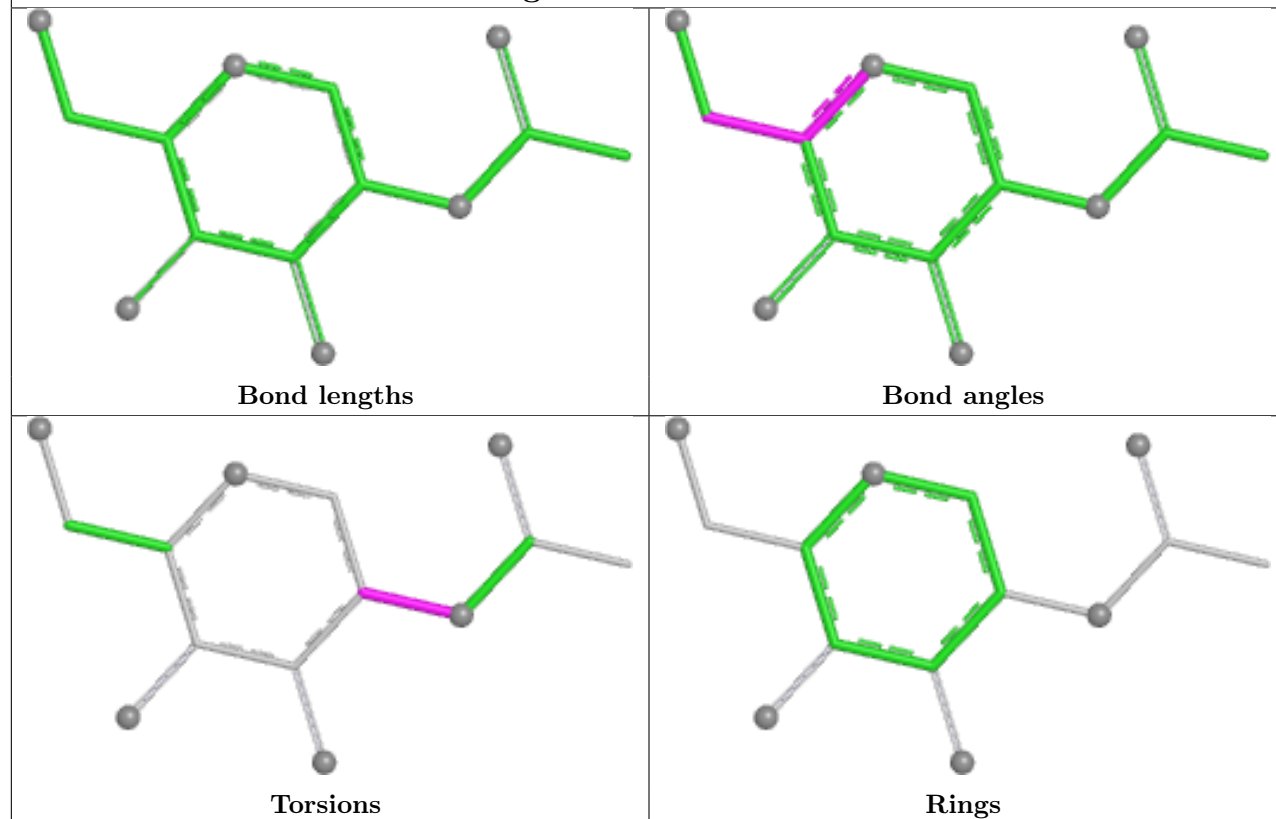
Ligand NAG F 1003



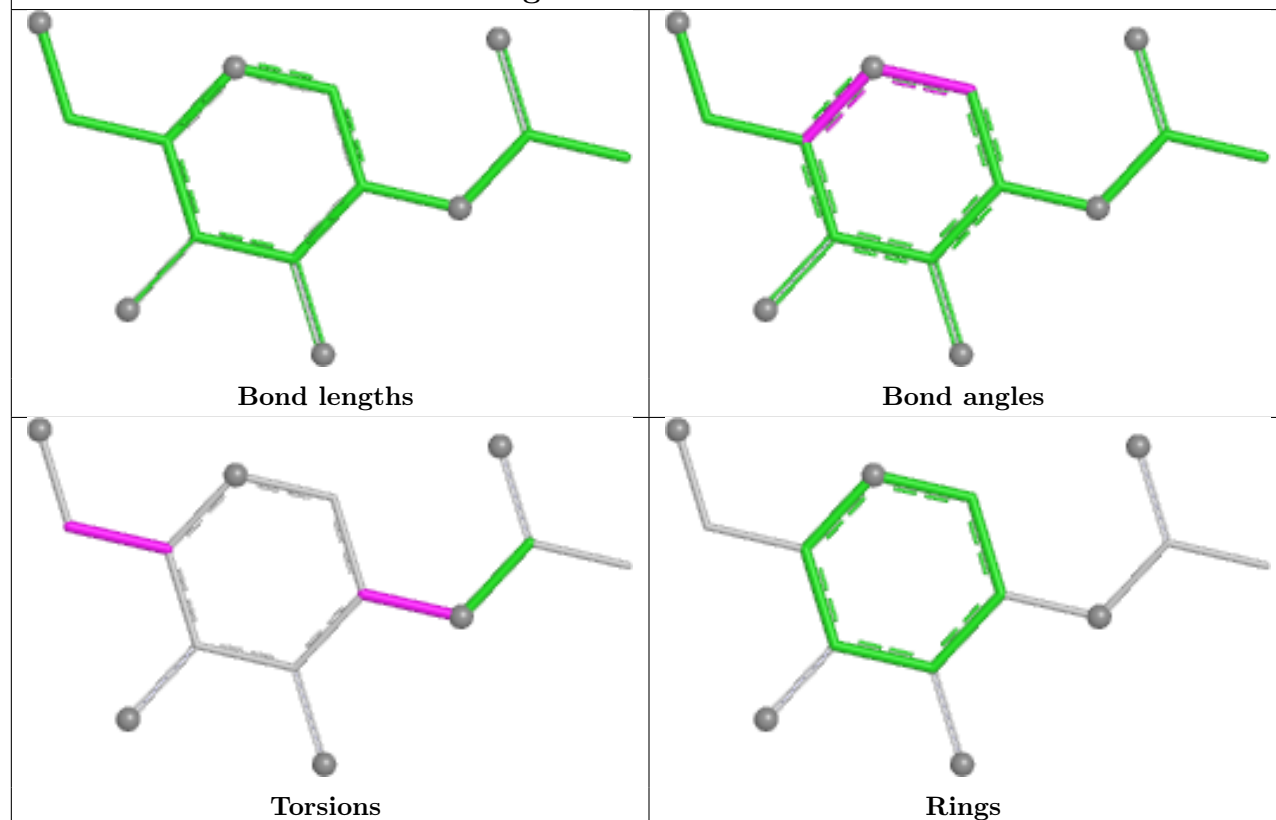
Ligand NAG K 503

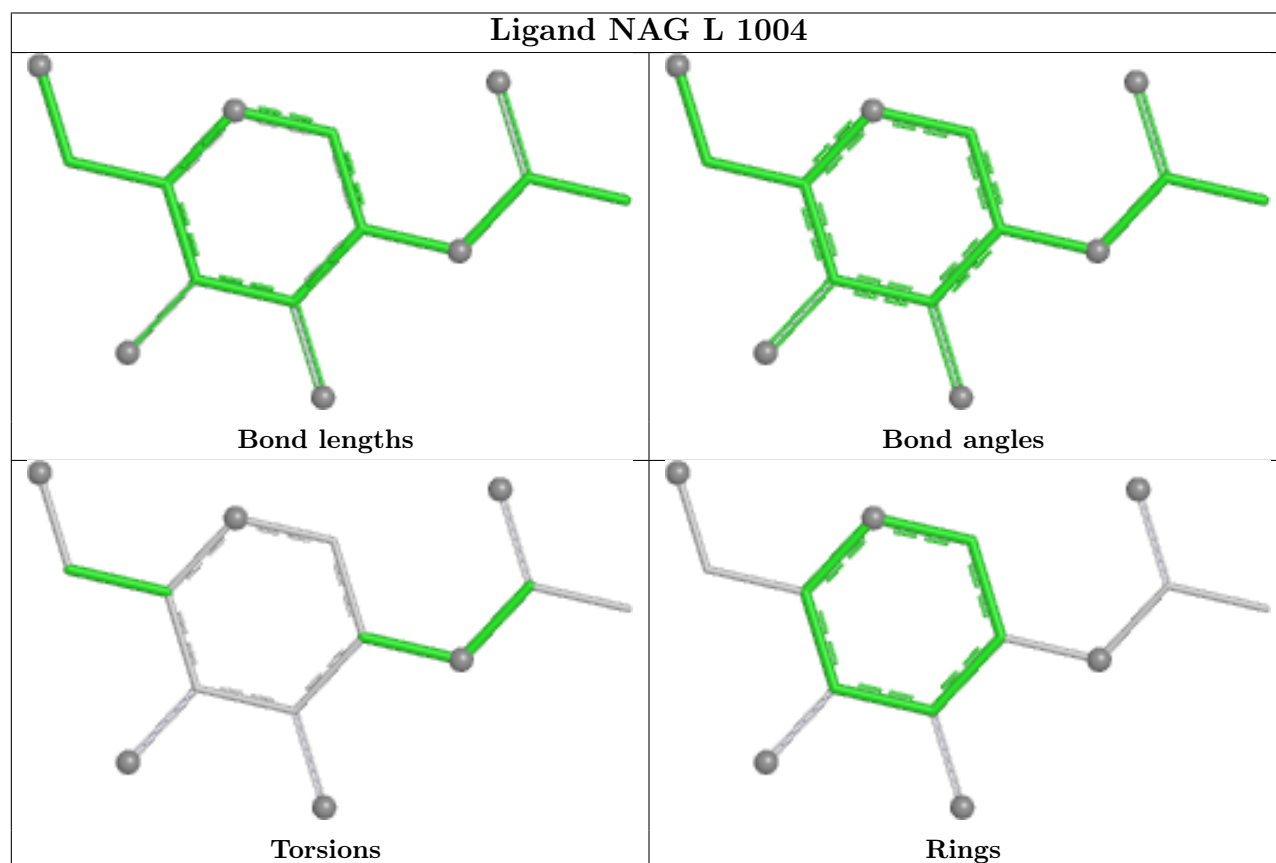
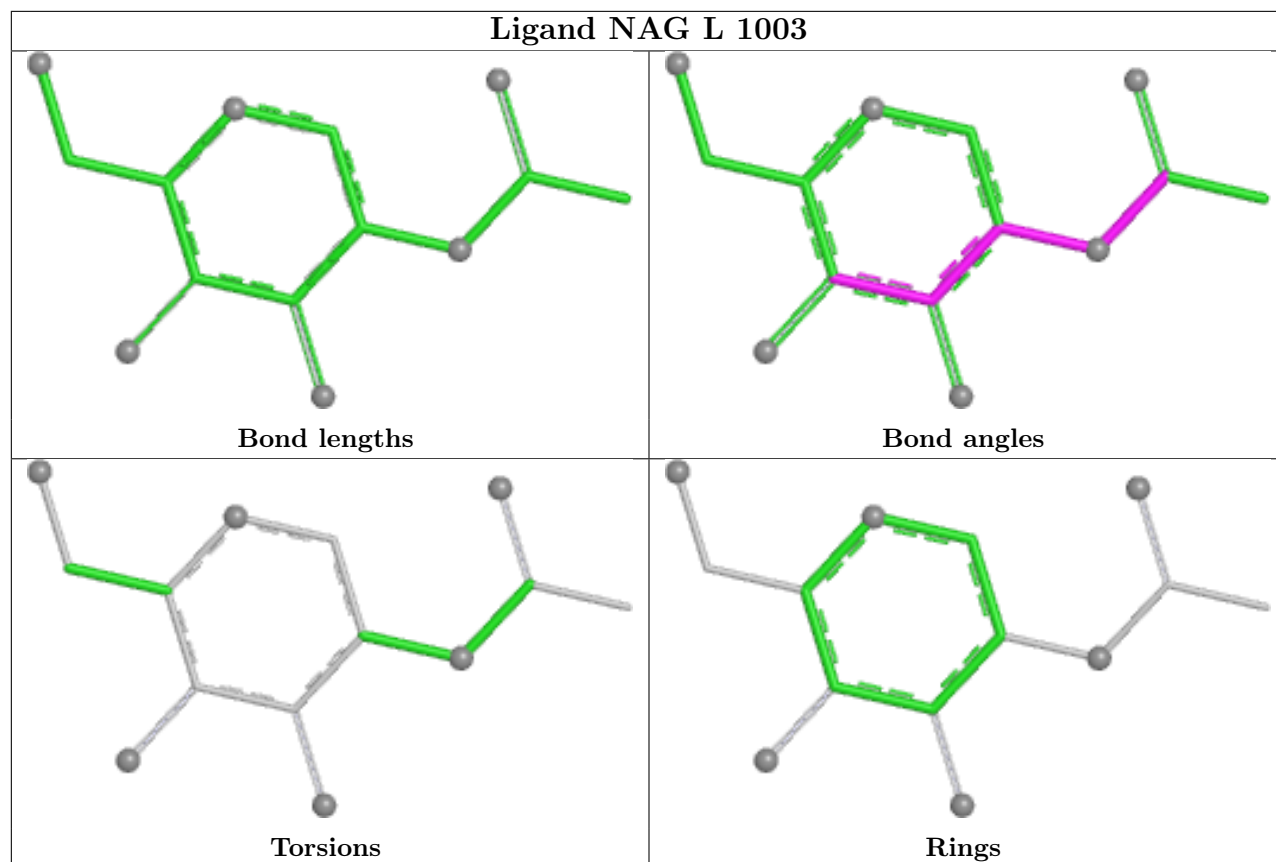


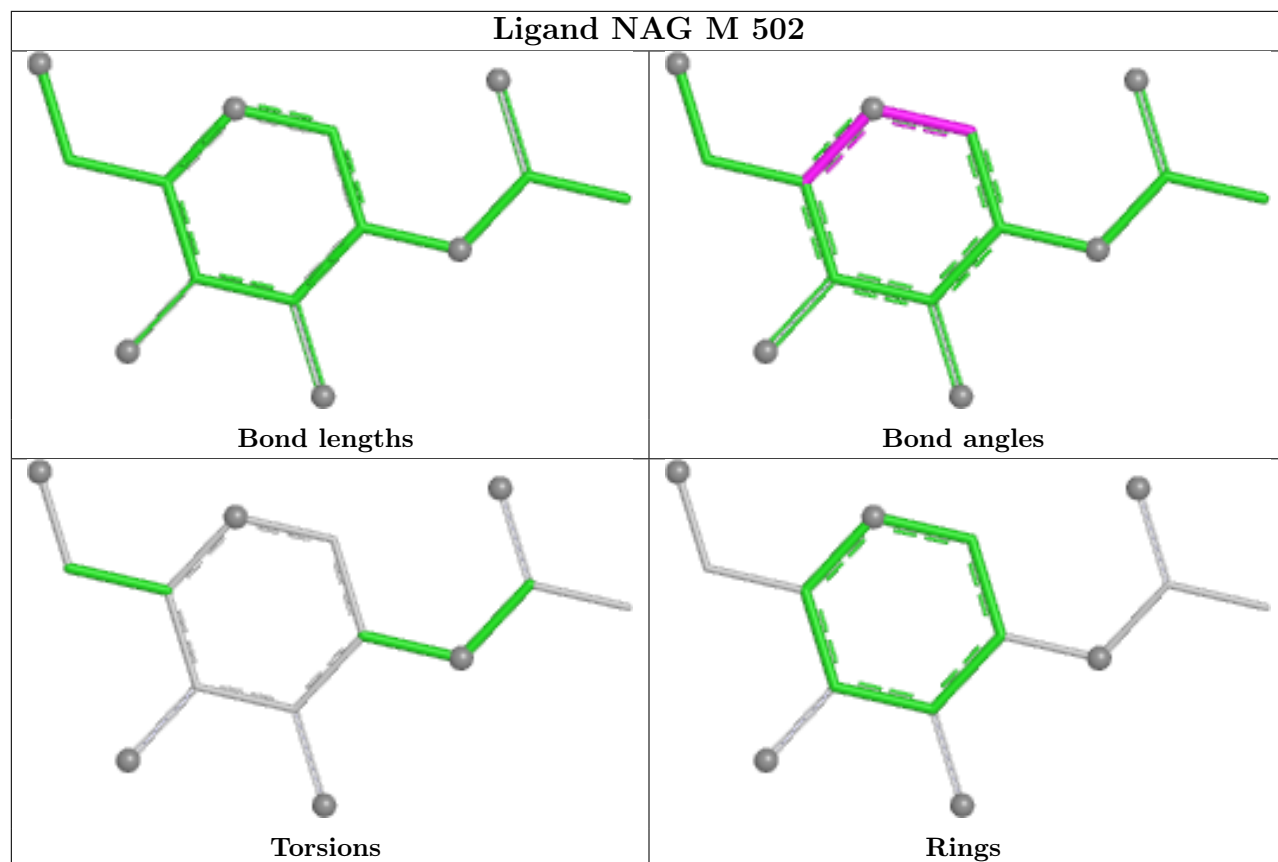
Ligand NAG J 1003

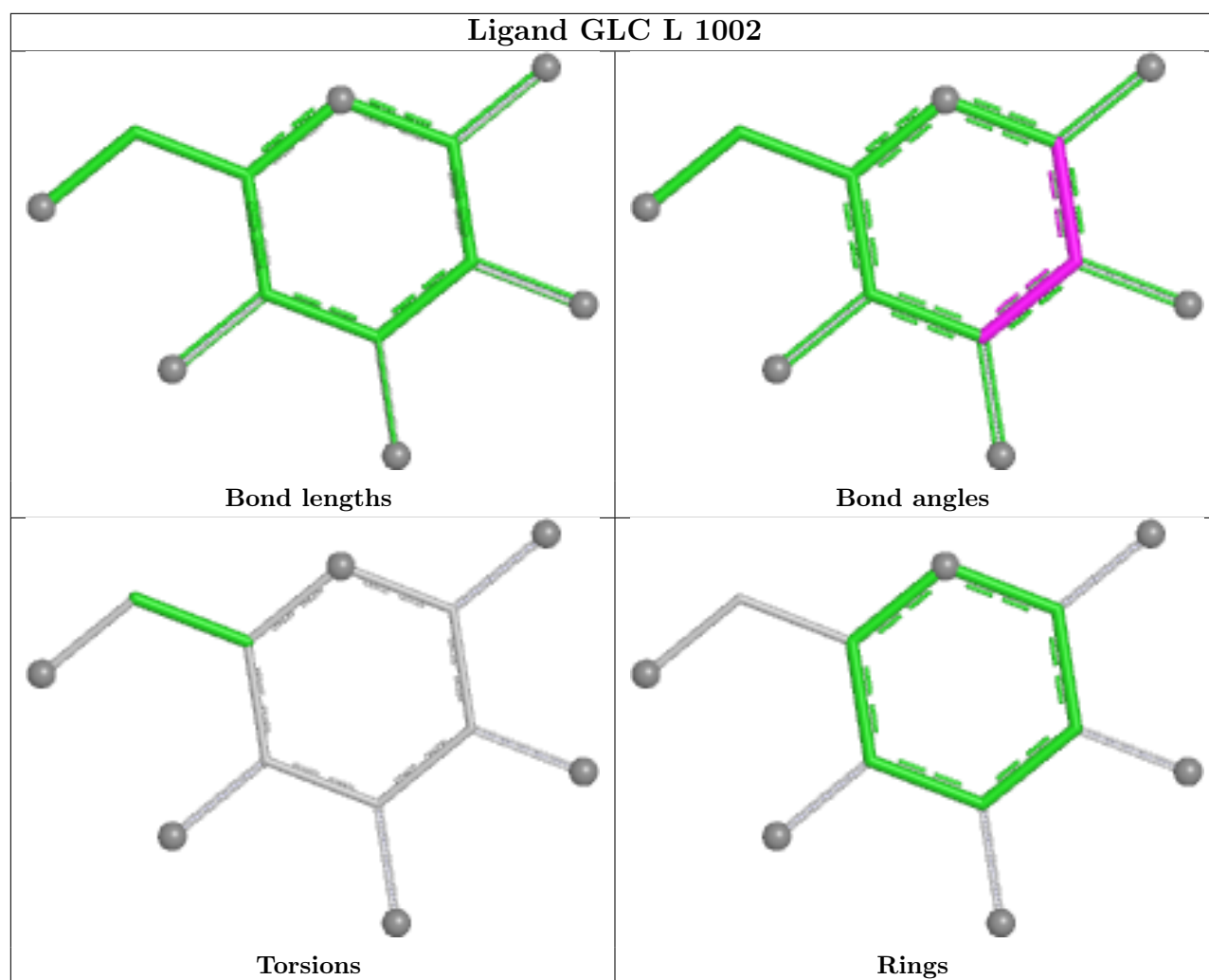


Ligand NAG J 1004

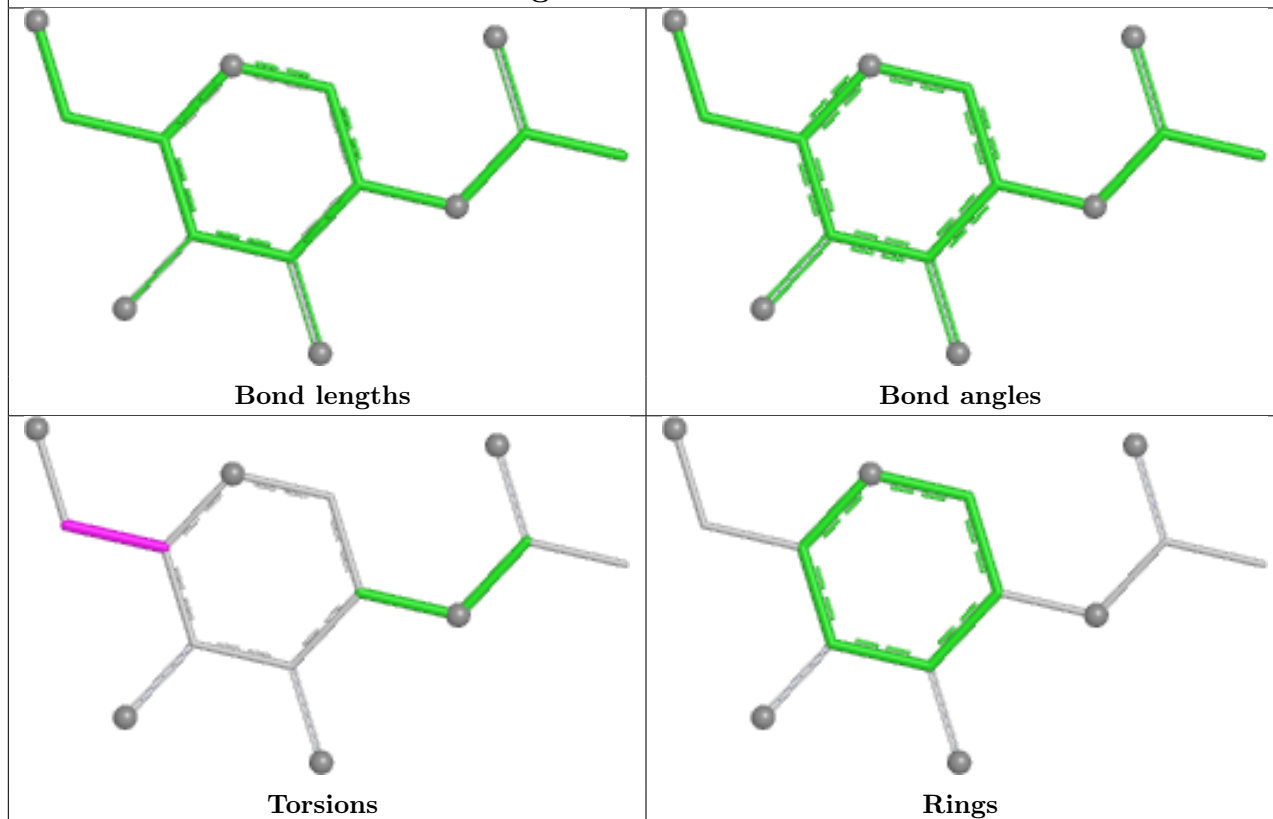




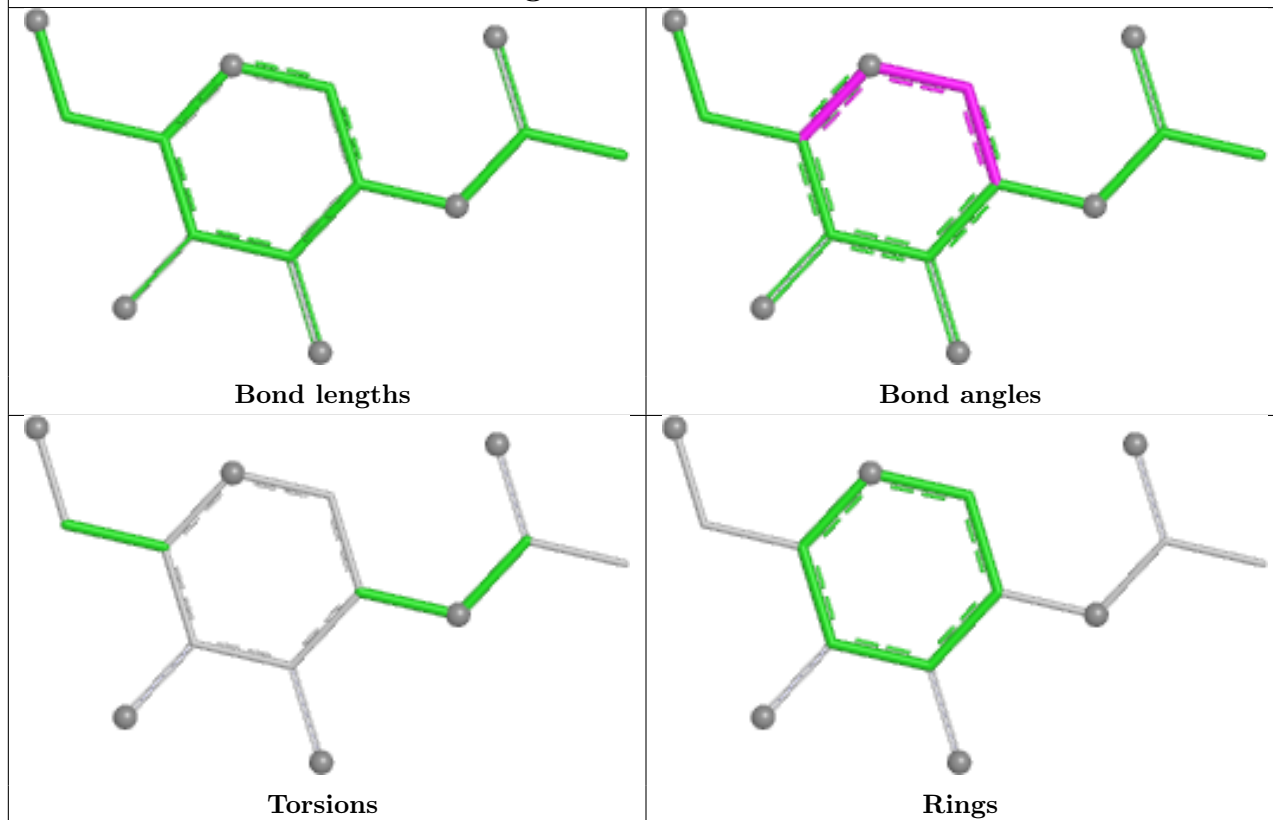


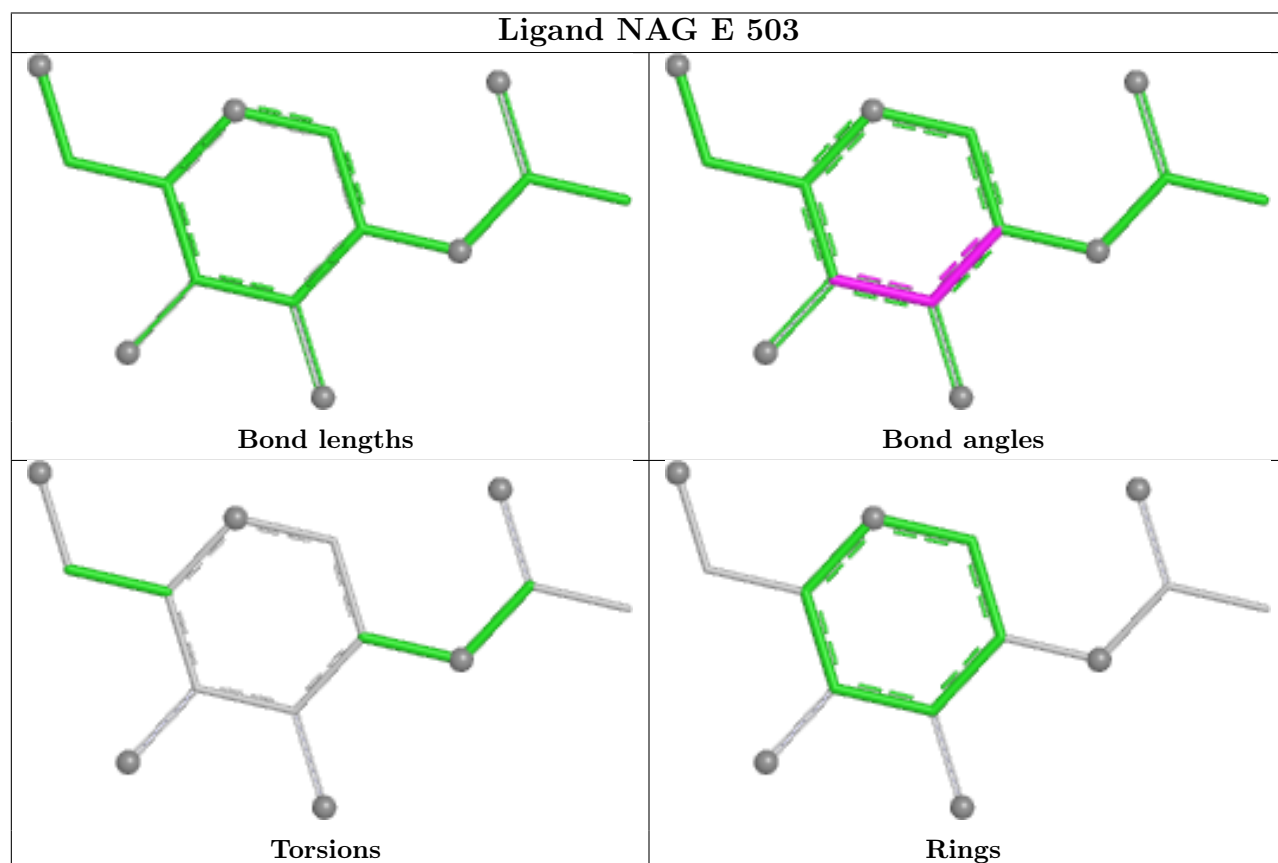
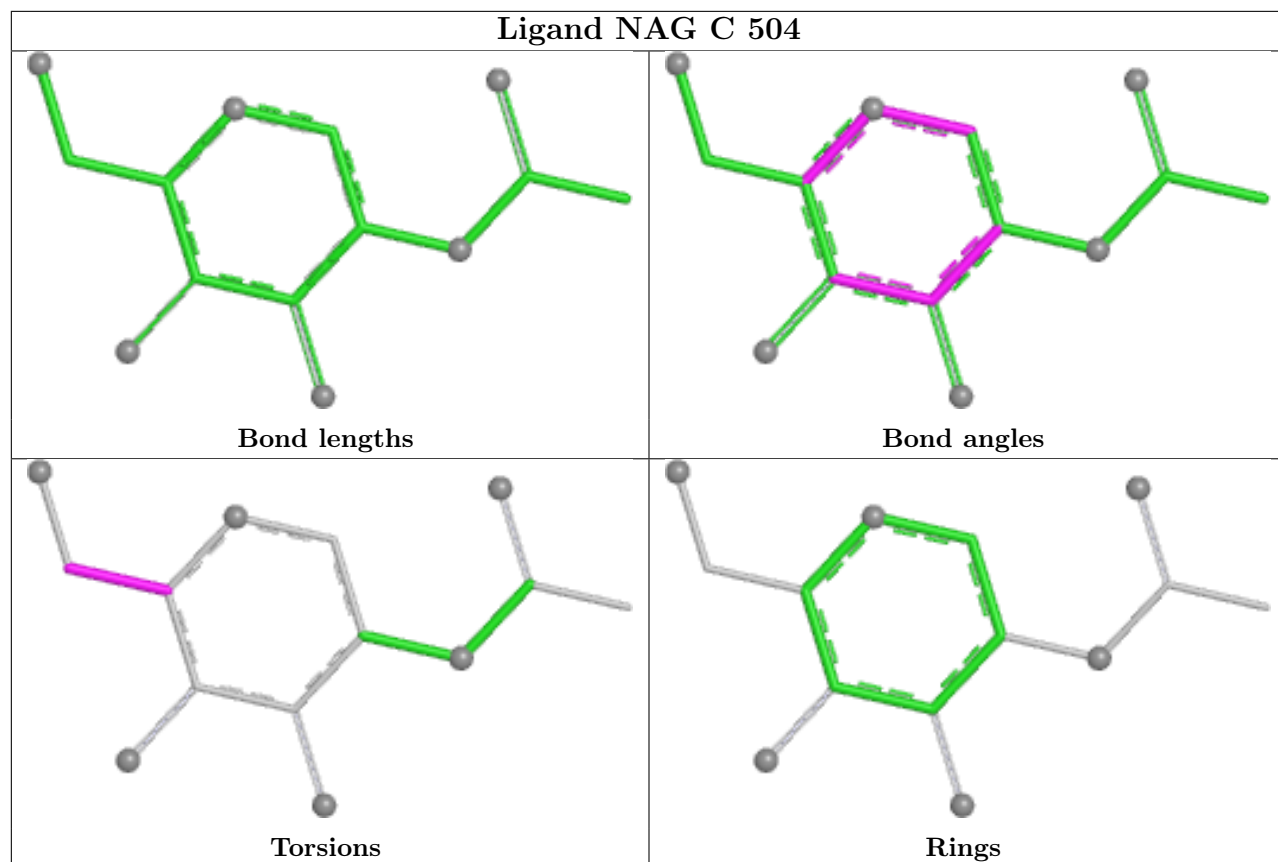


Ligand NAG I 505

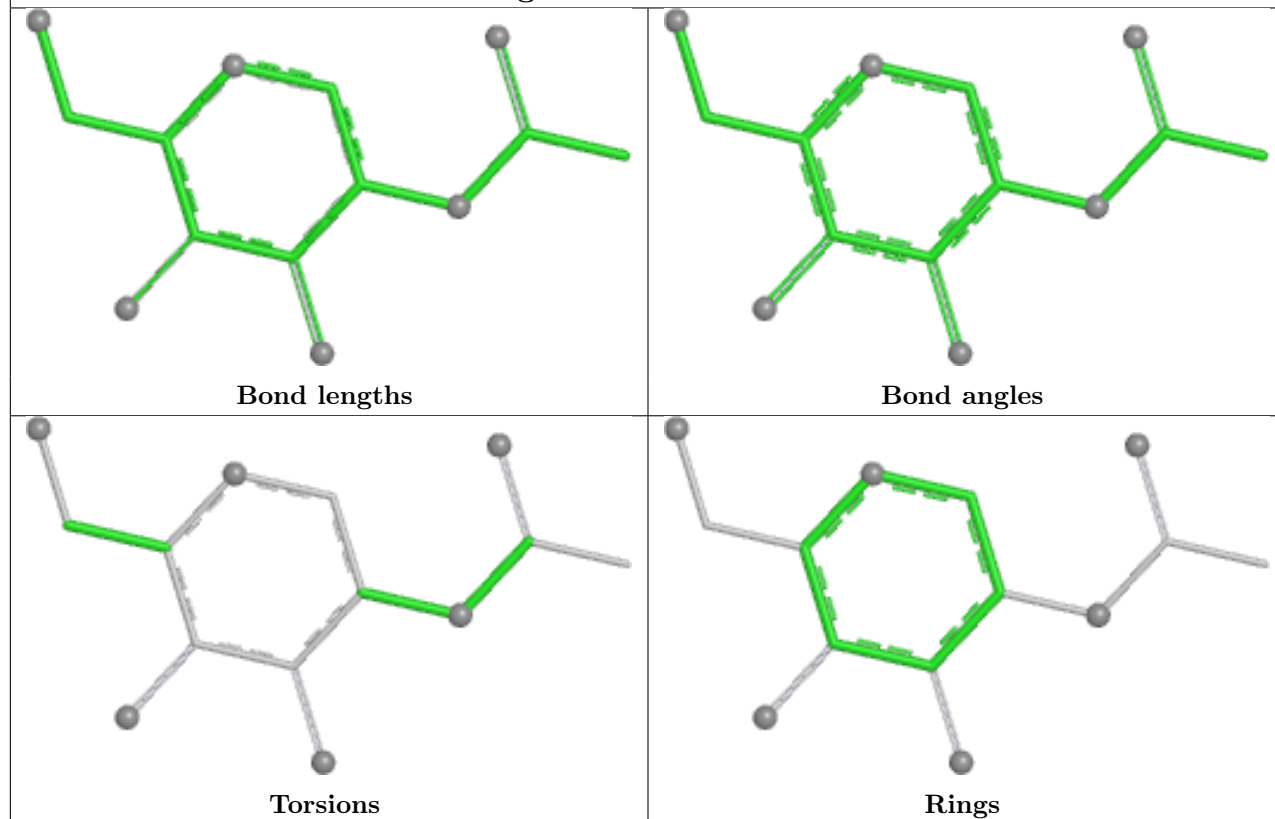


Ligand NAG G 505

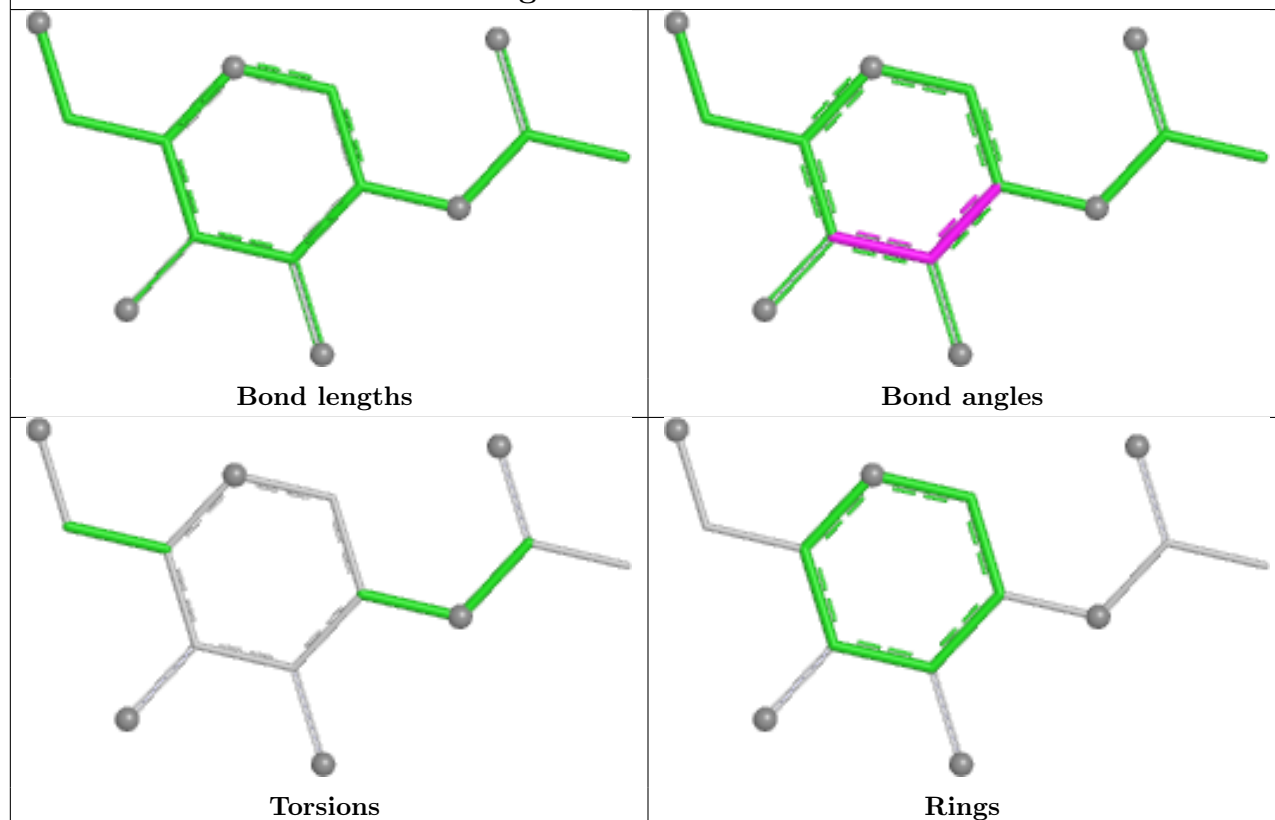


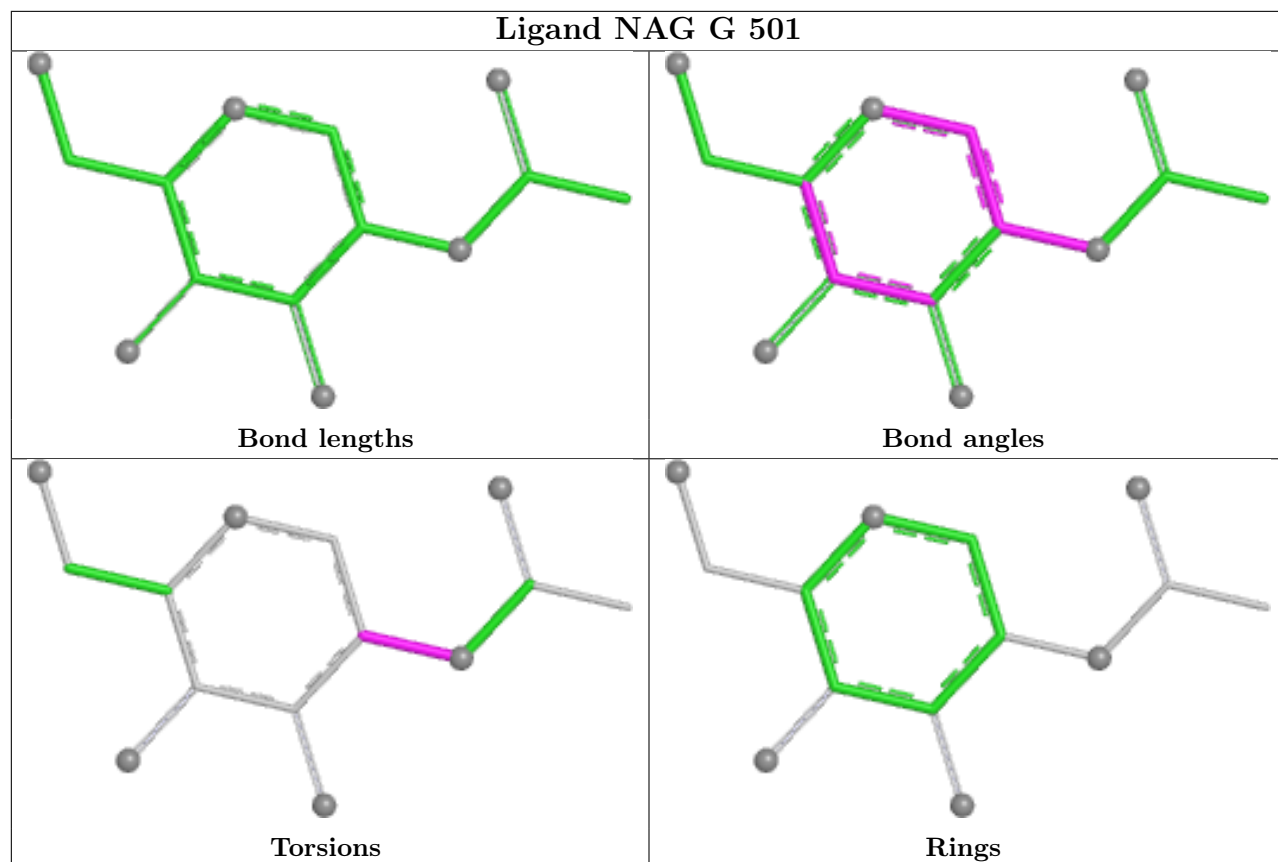


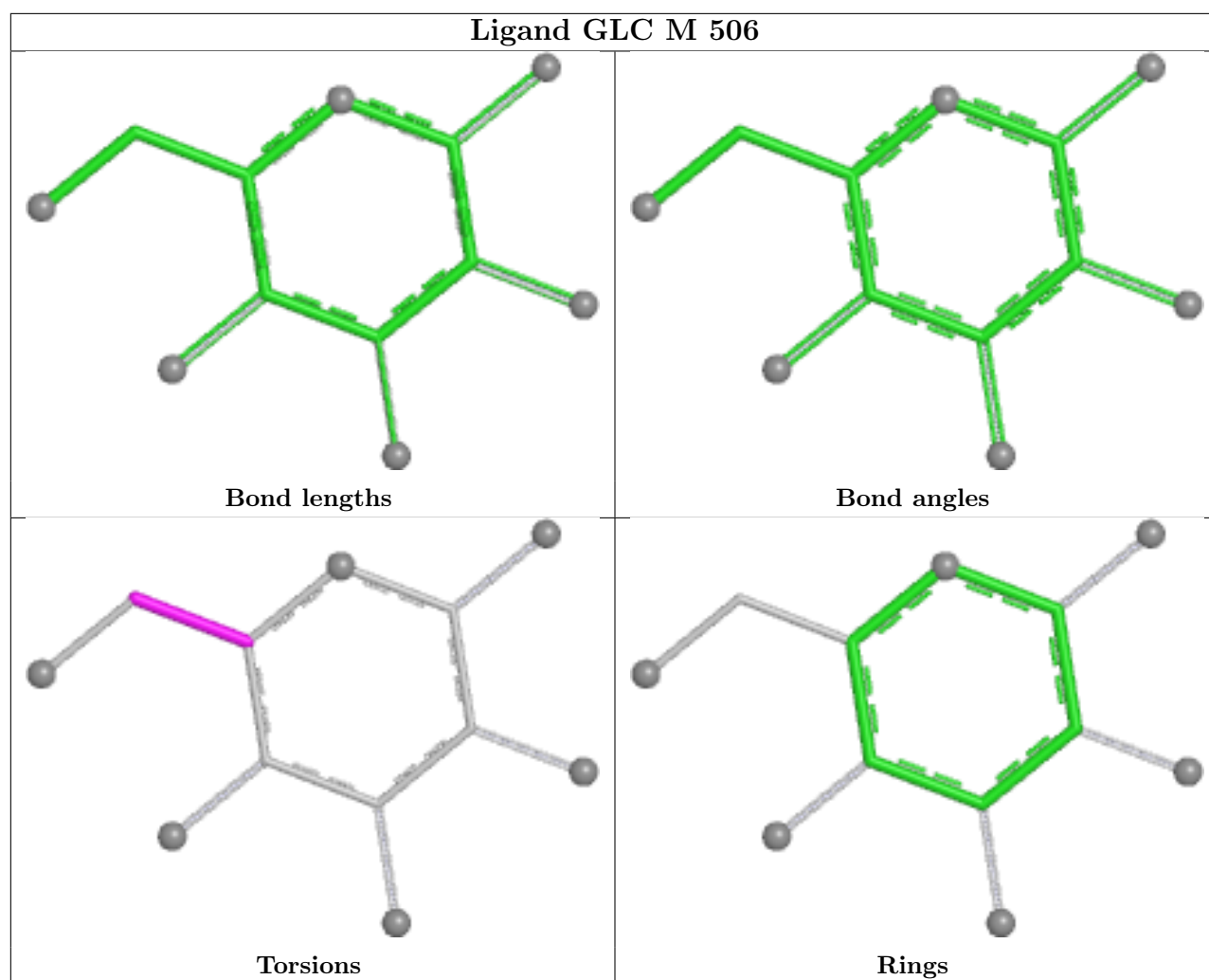
Ligand NAG N 1002

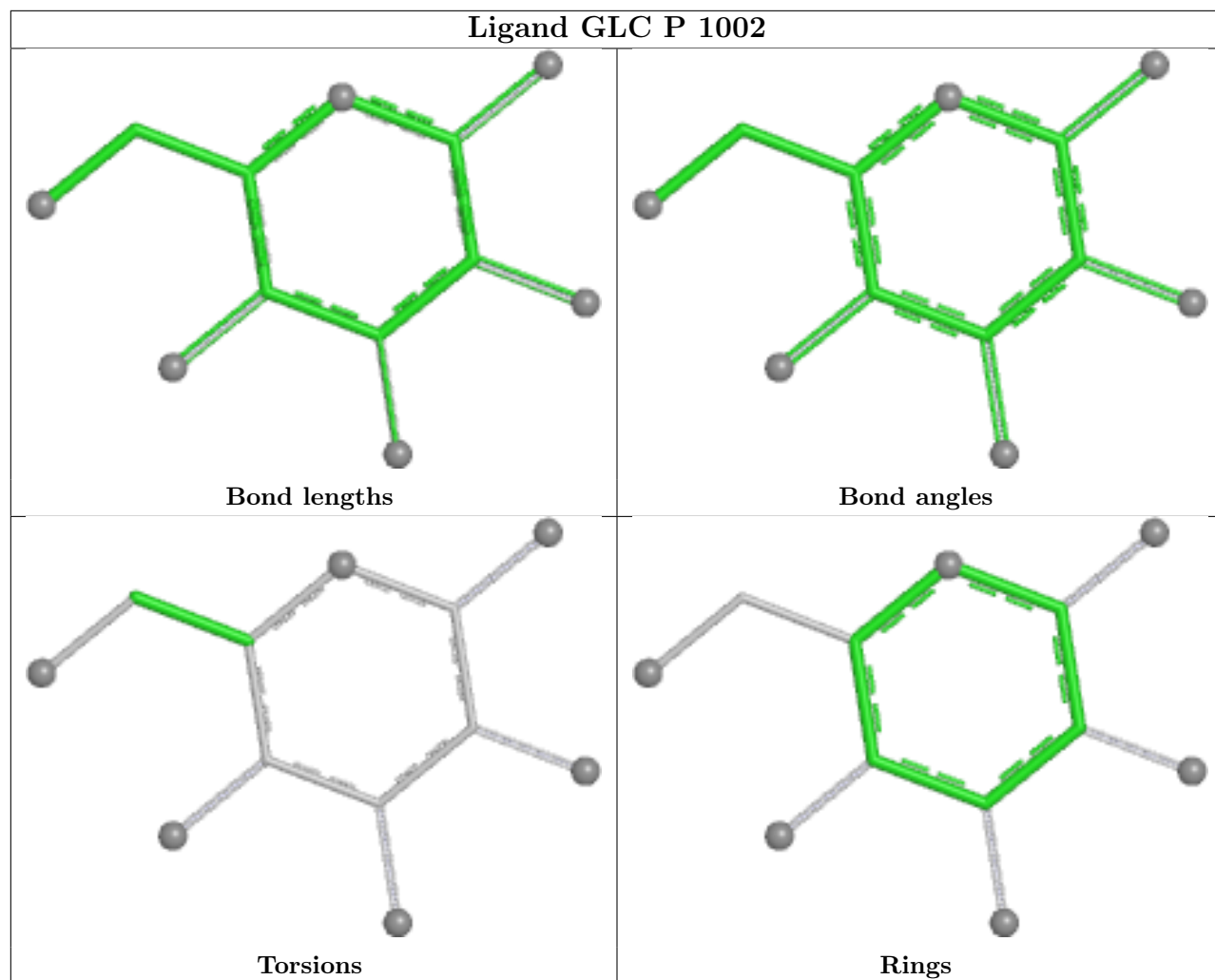


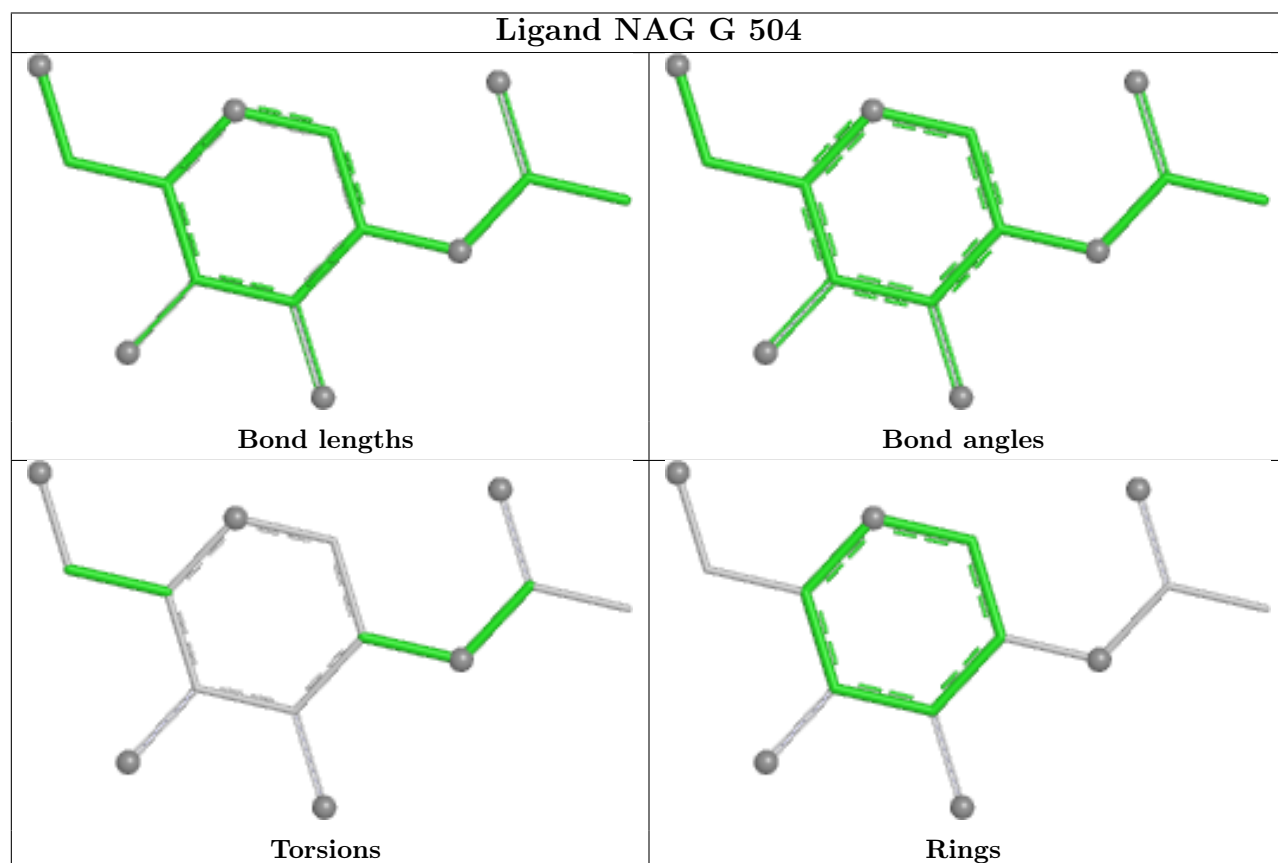
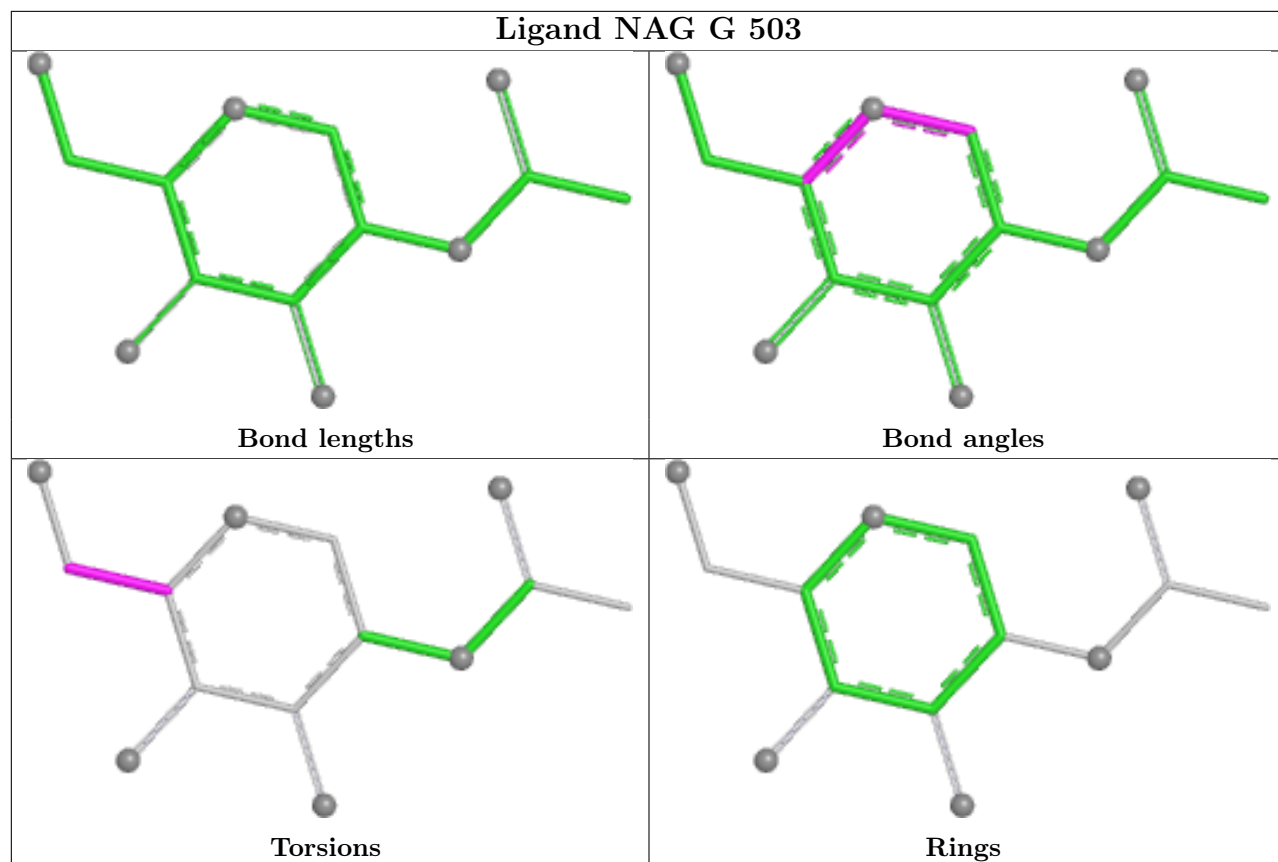
Ligand NAG P 1003



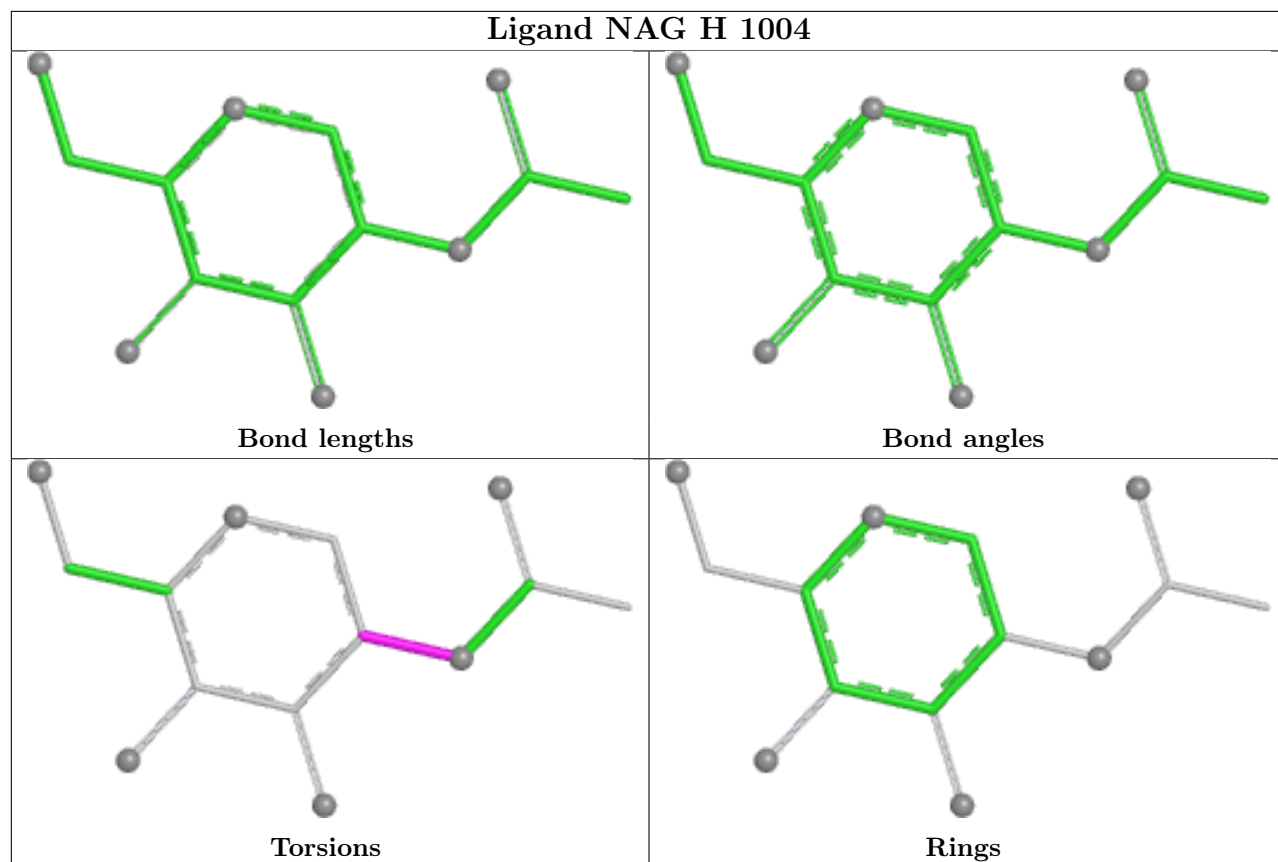




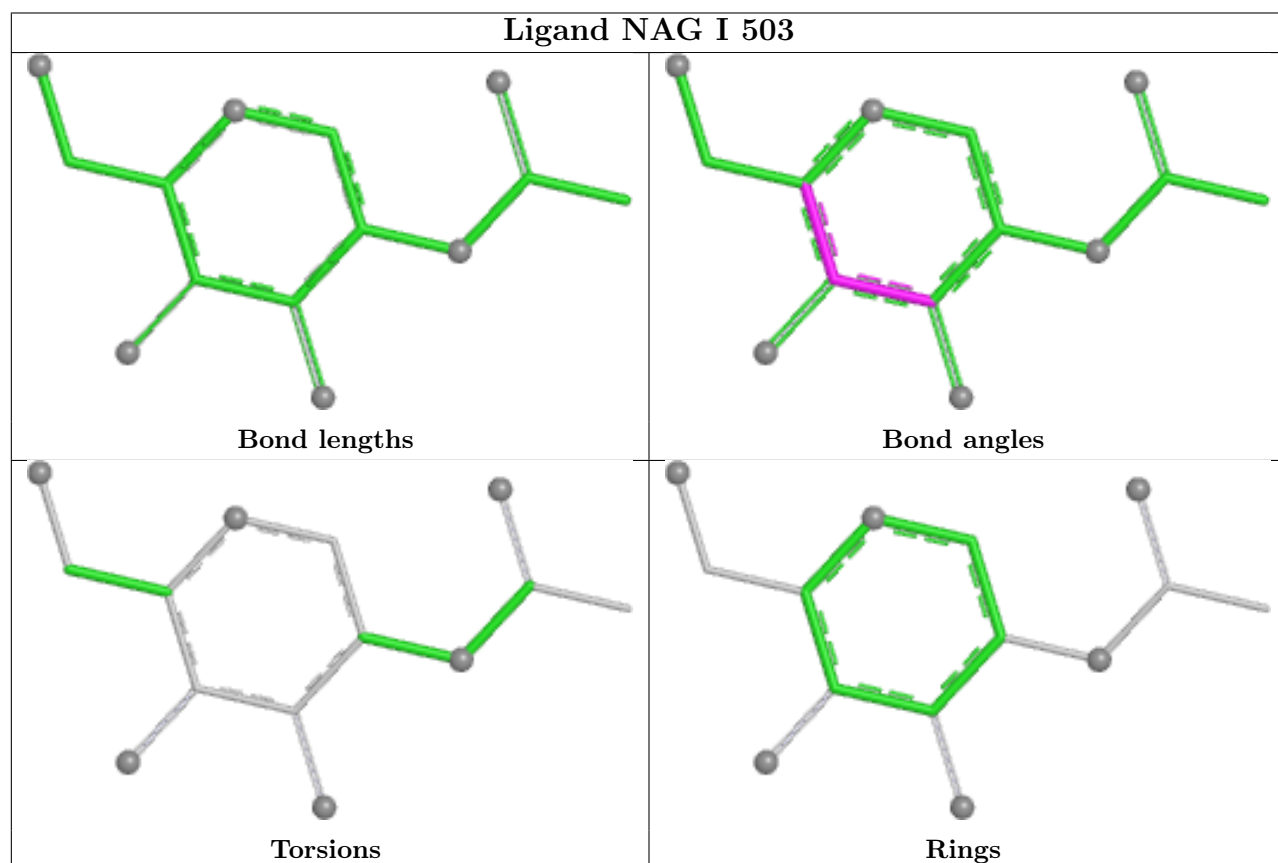


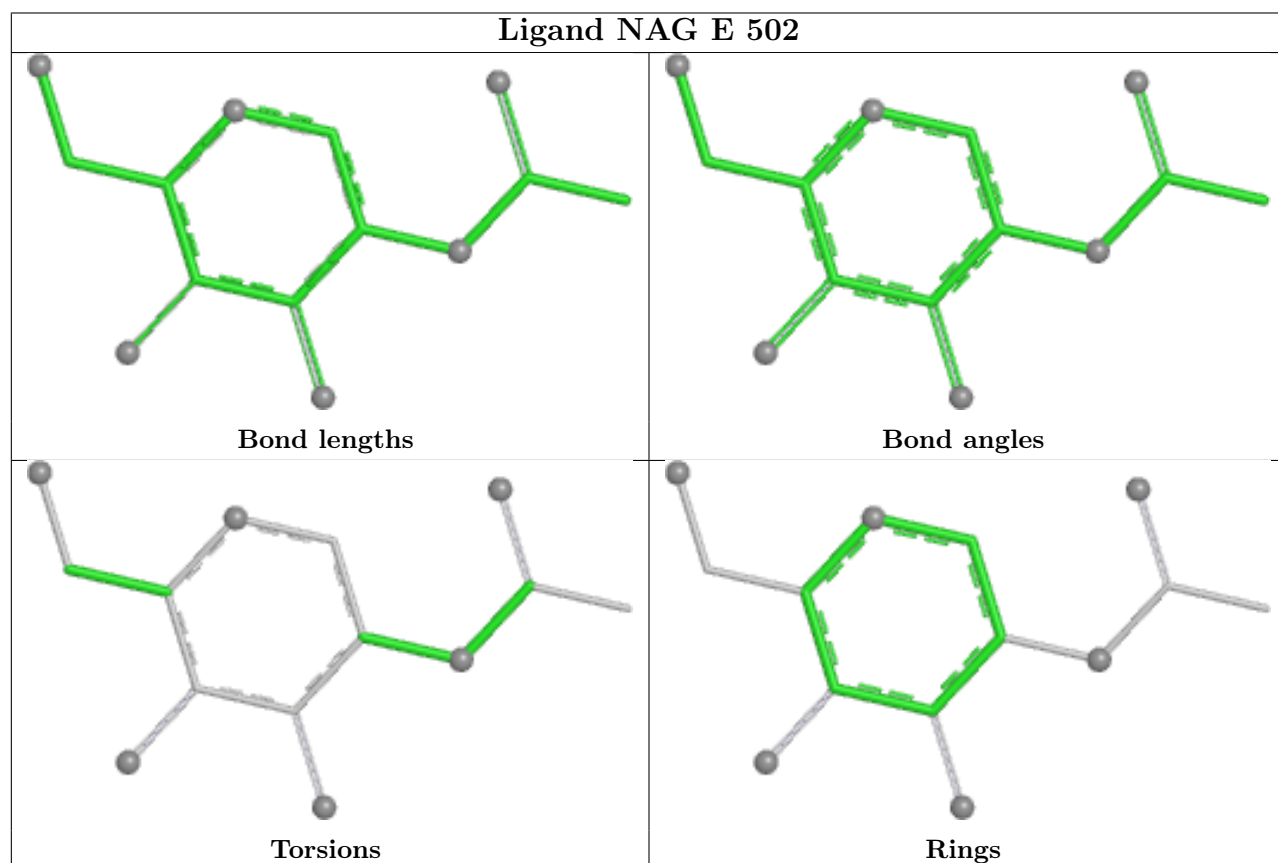
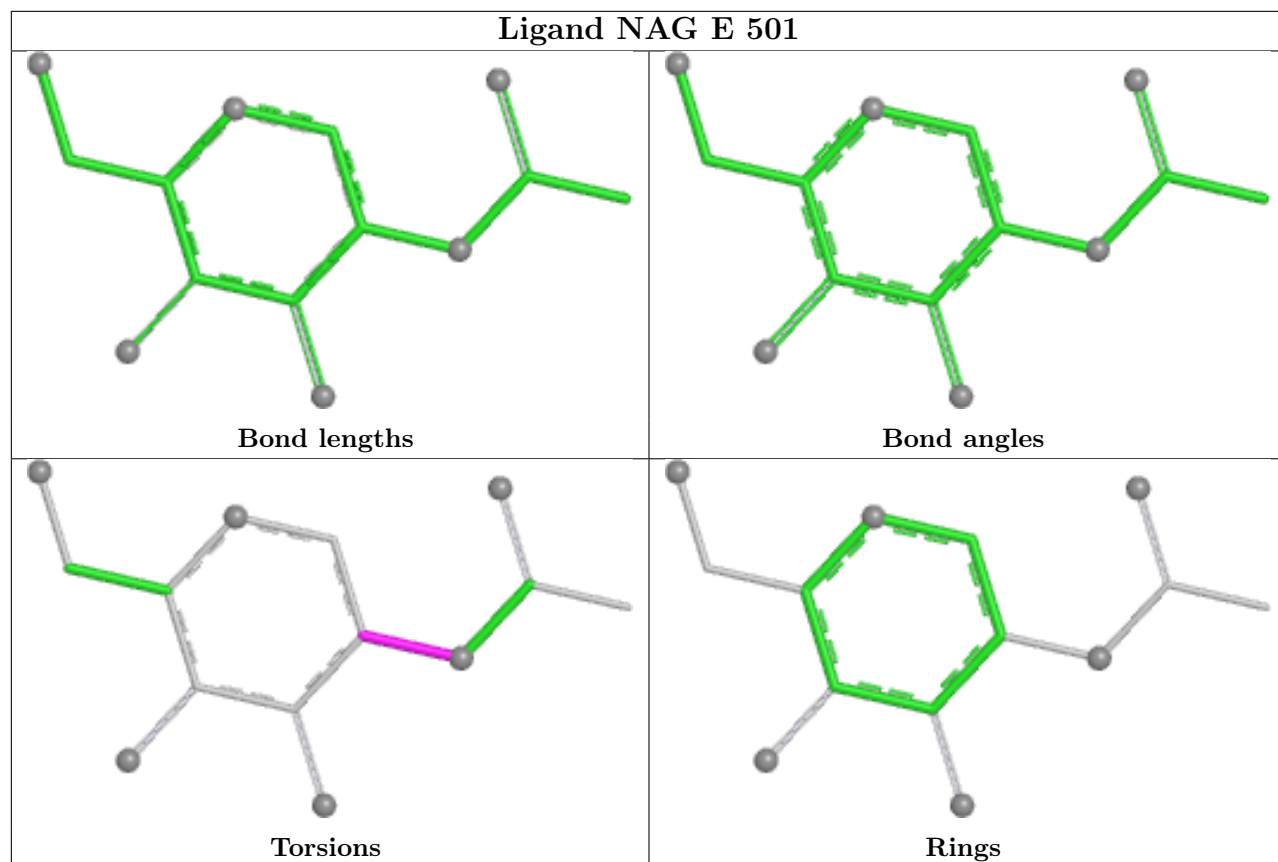


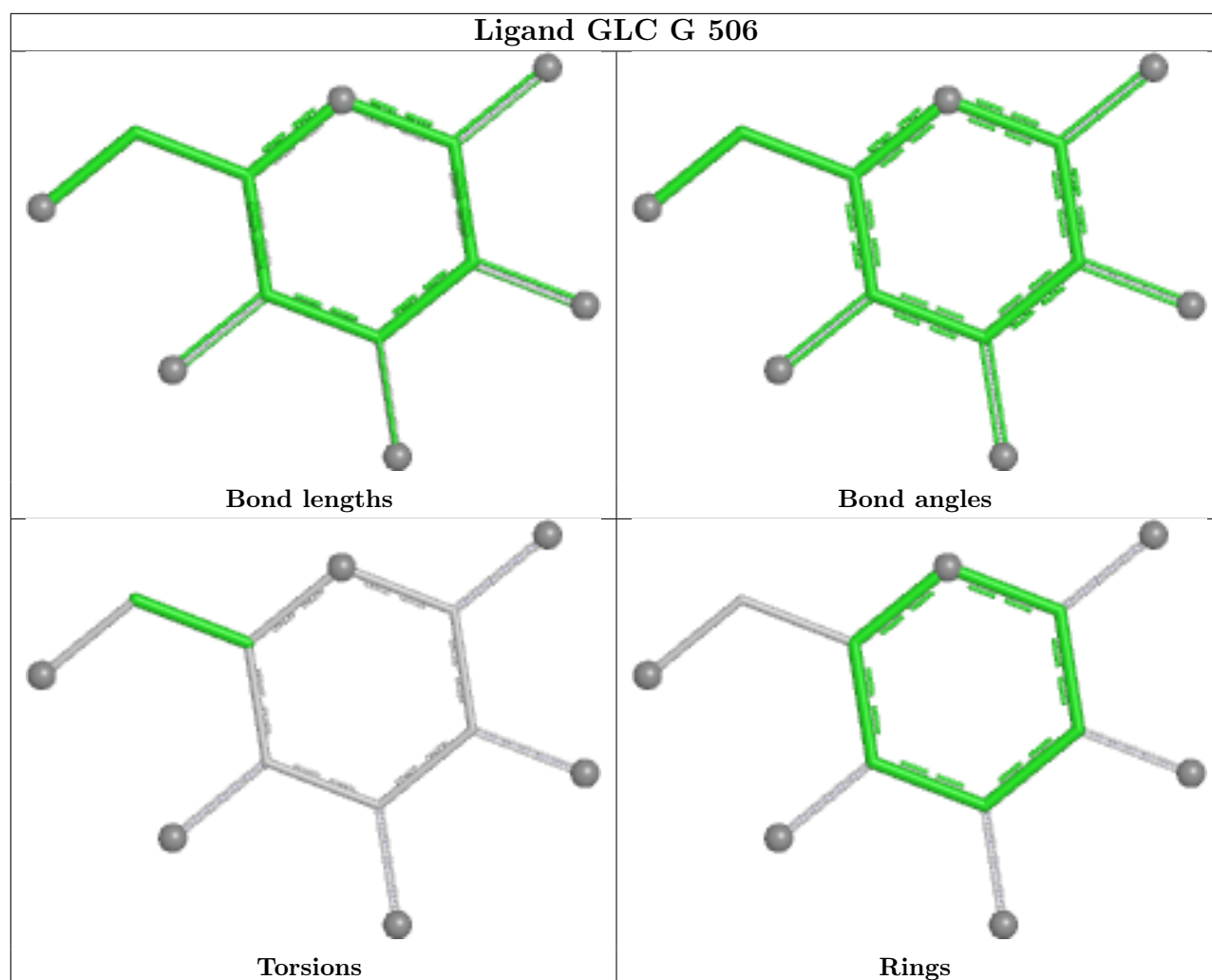
Ligand NAG H 1004

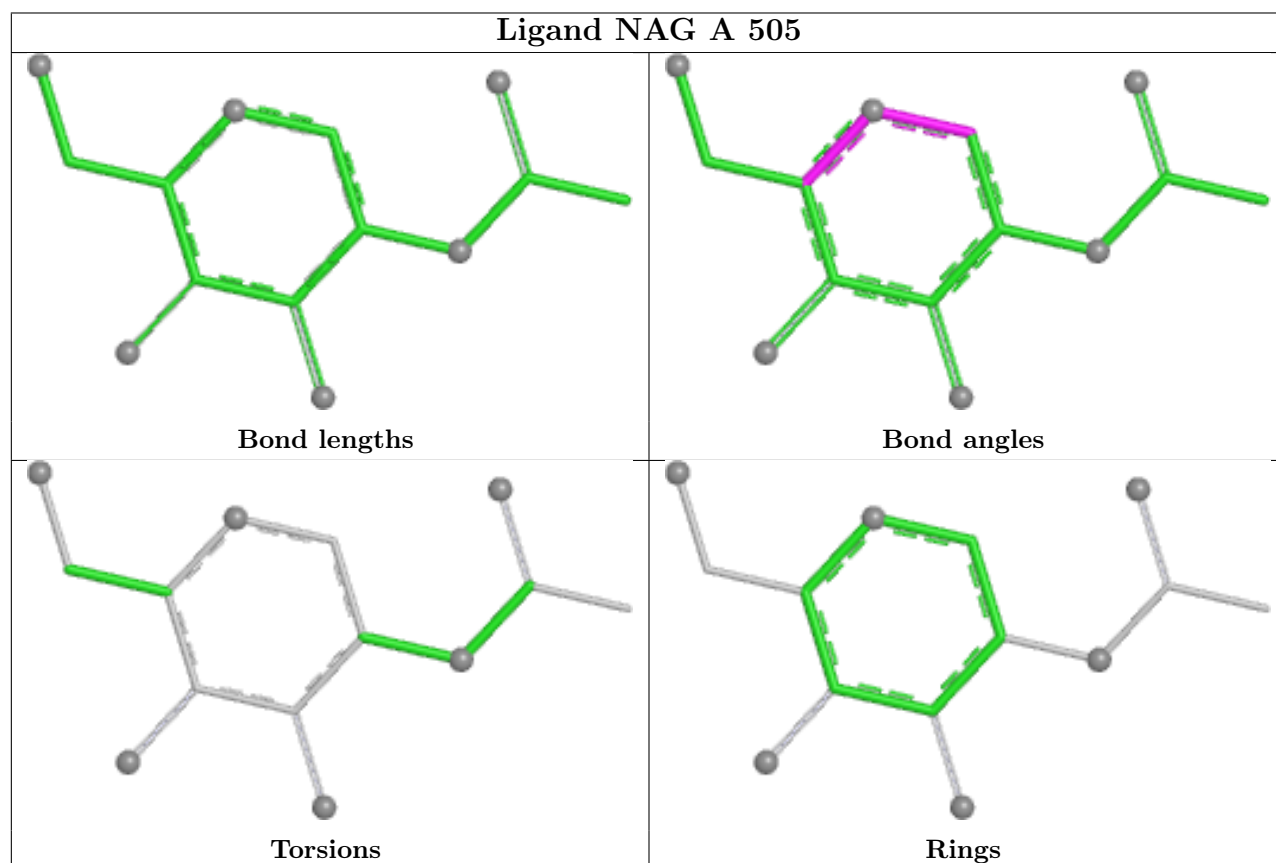
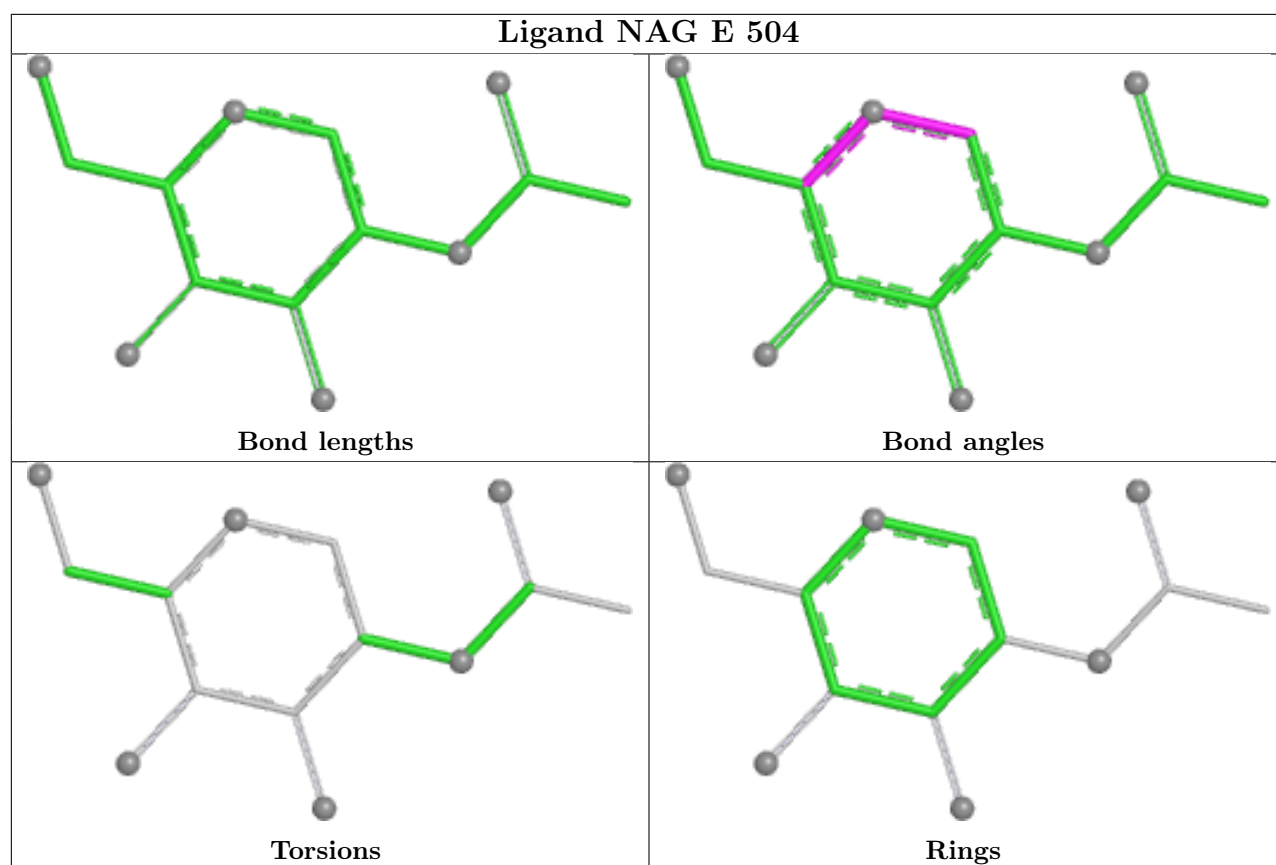


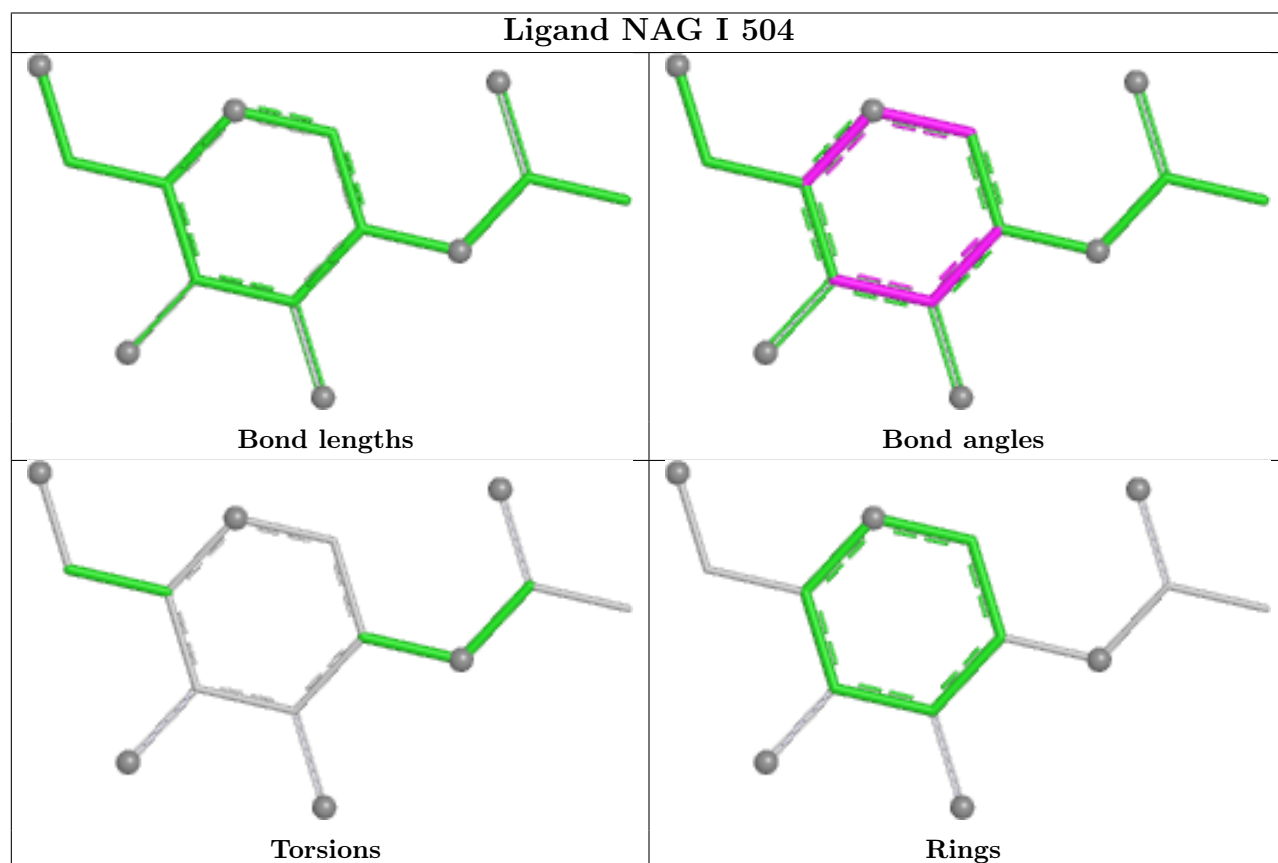
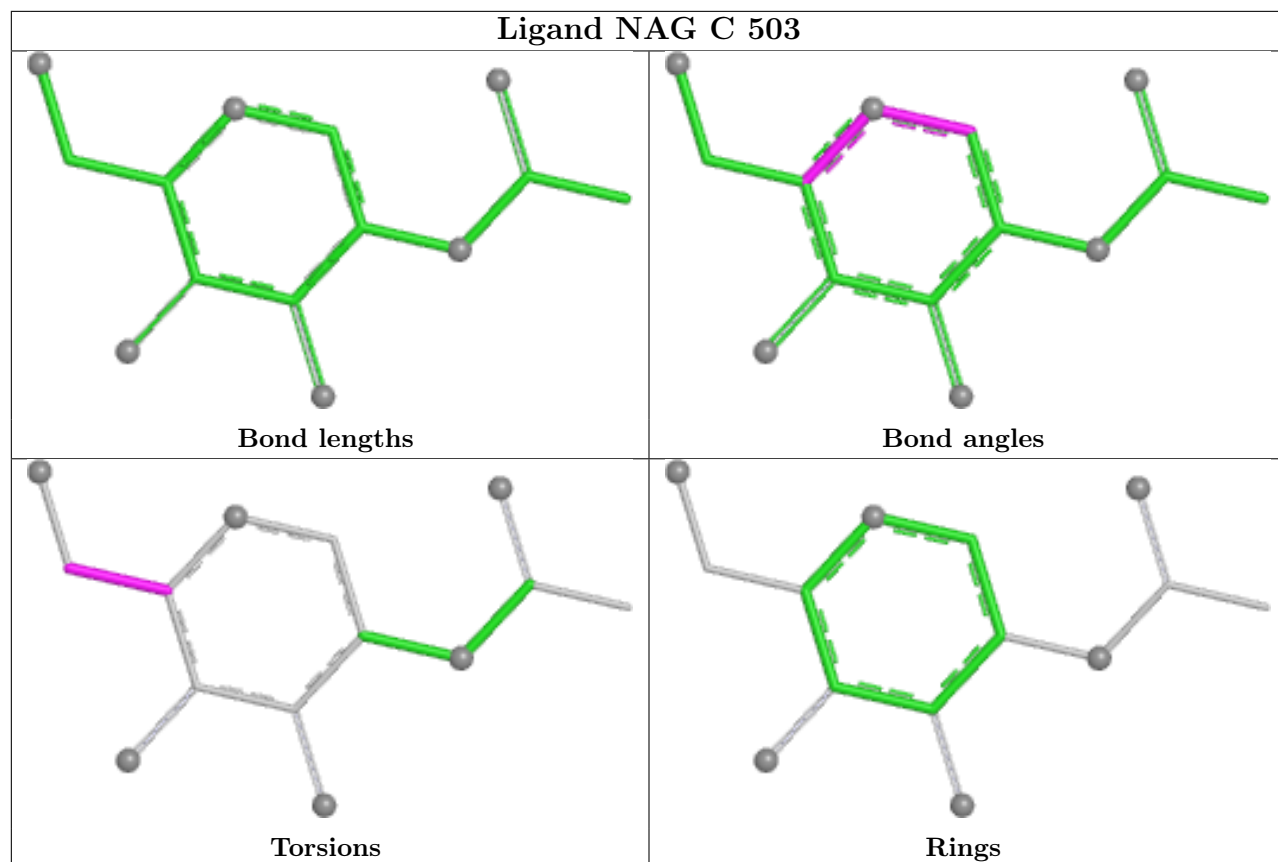
Ligand NAG I 503

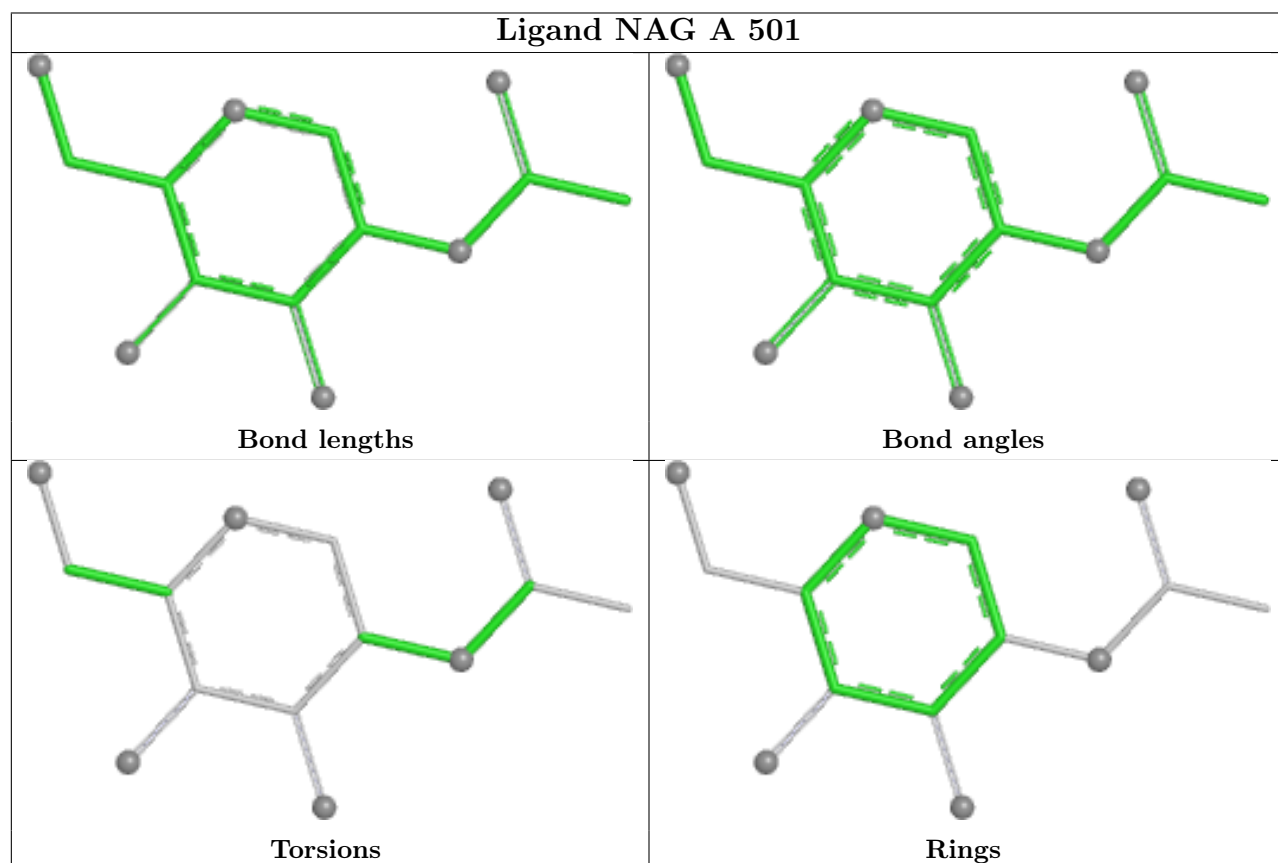
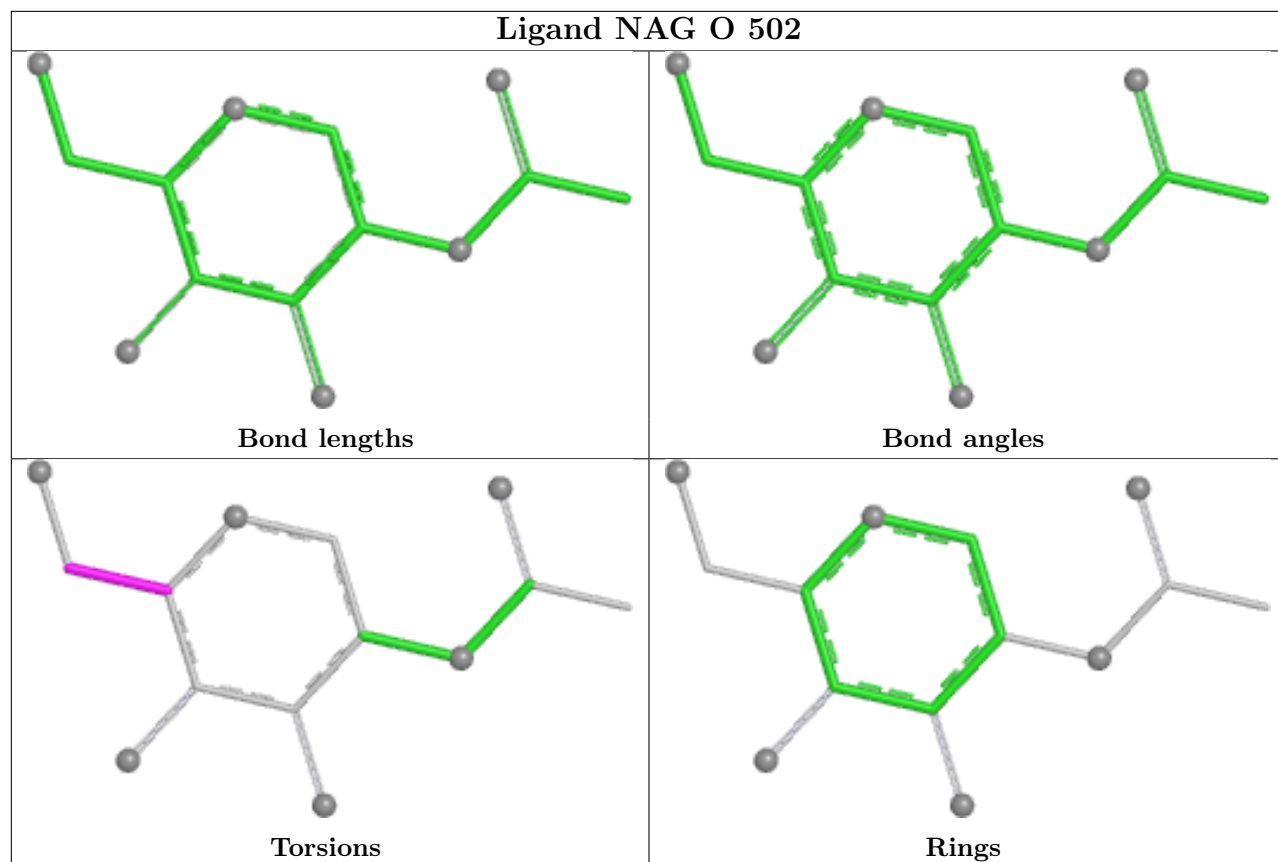


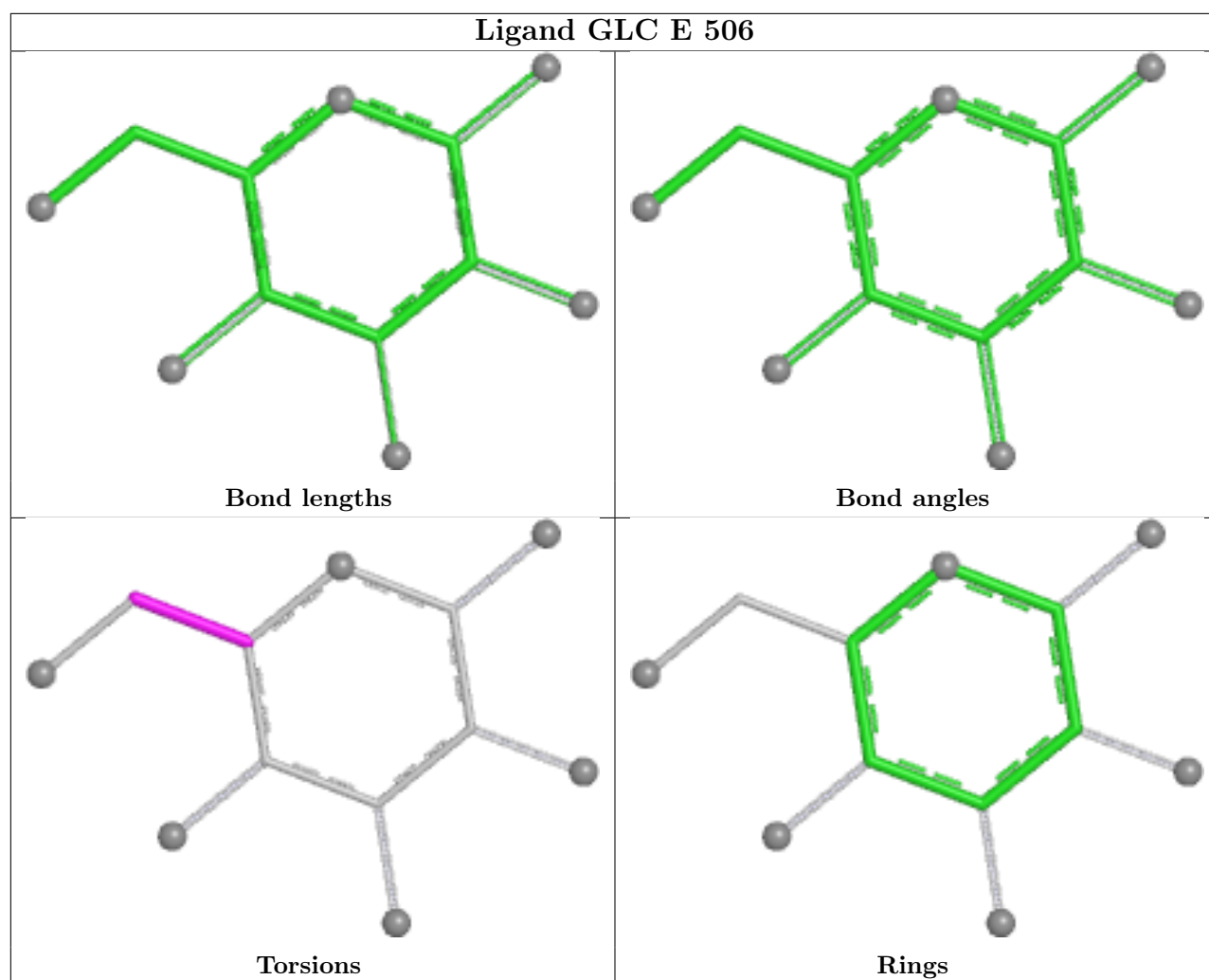


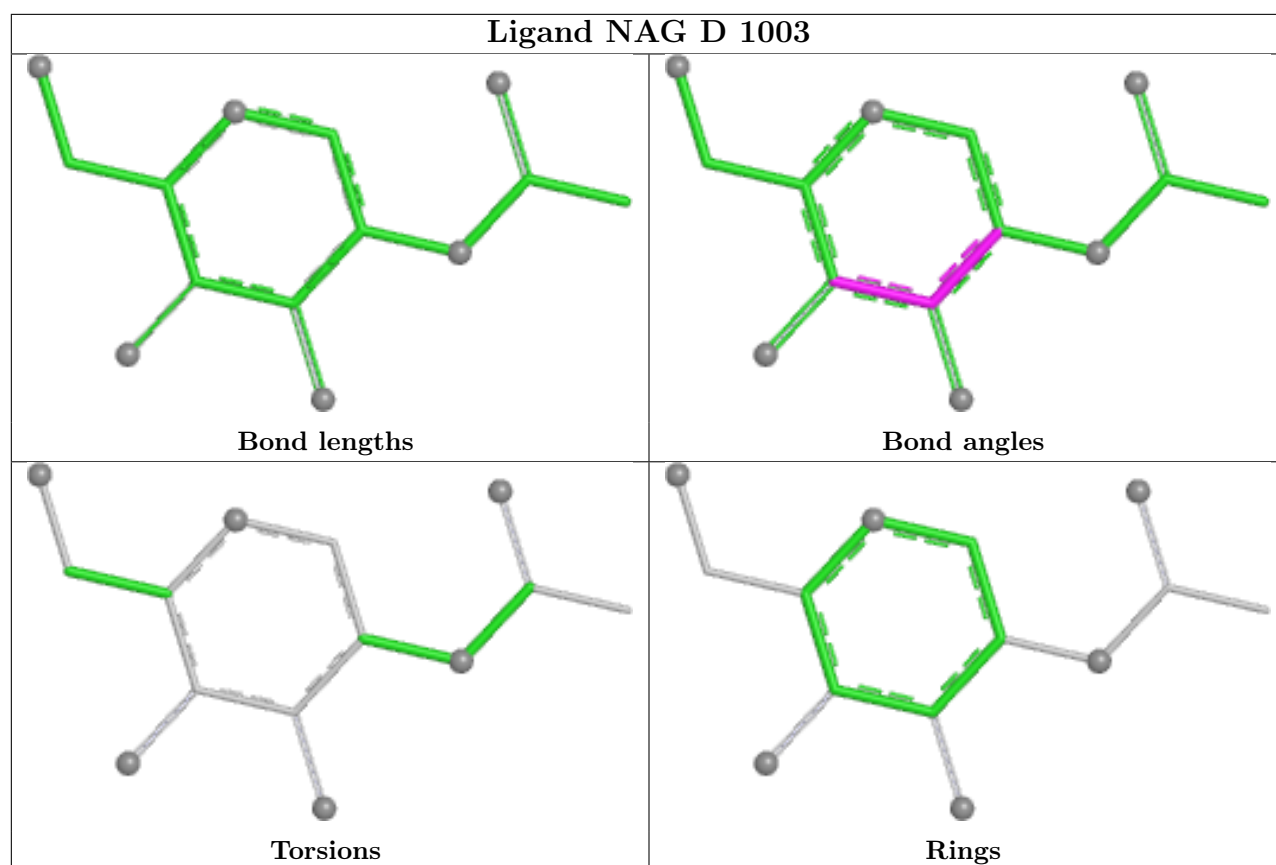


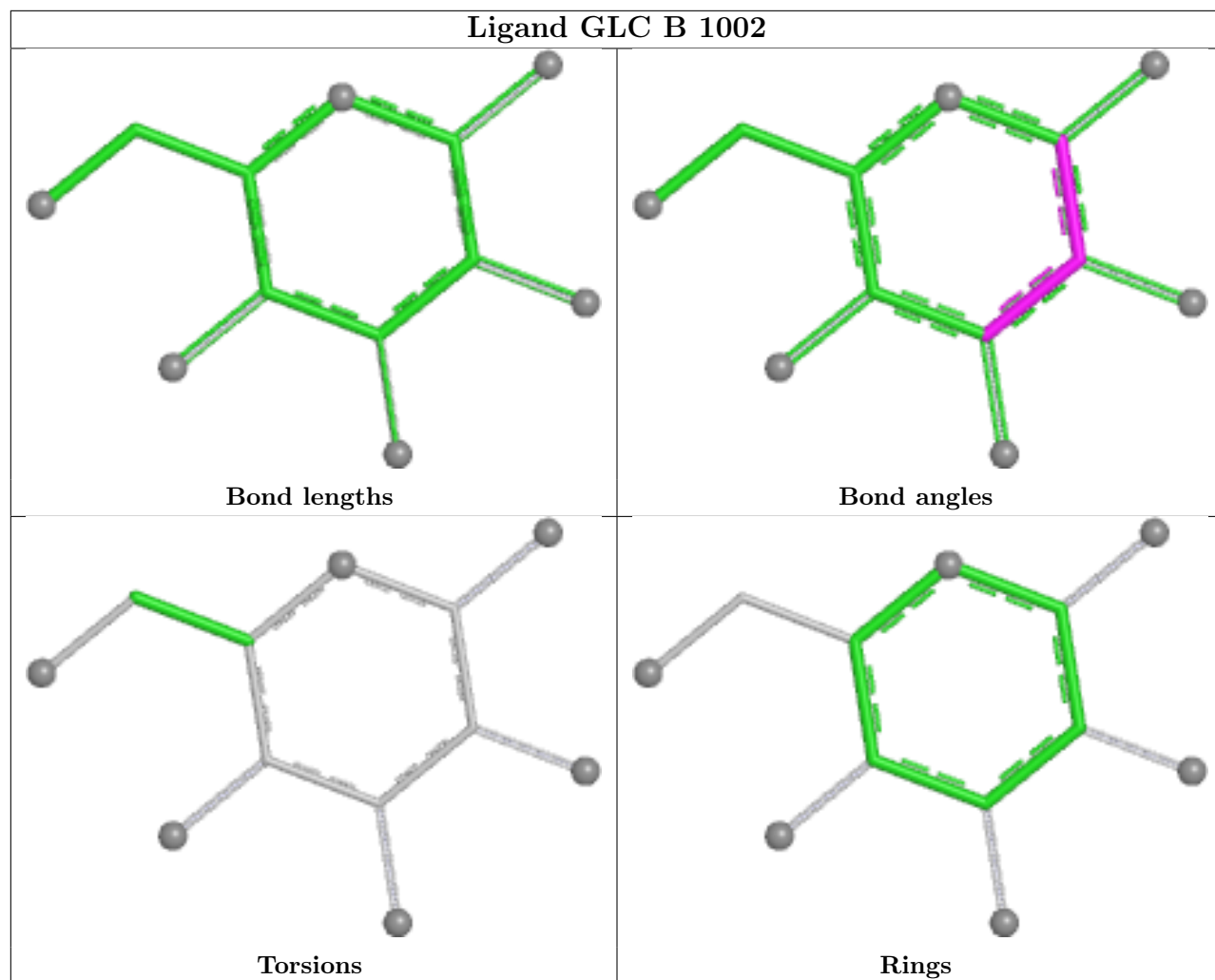




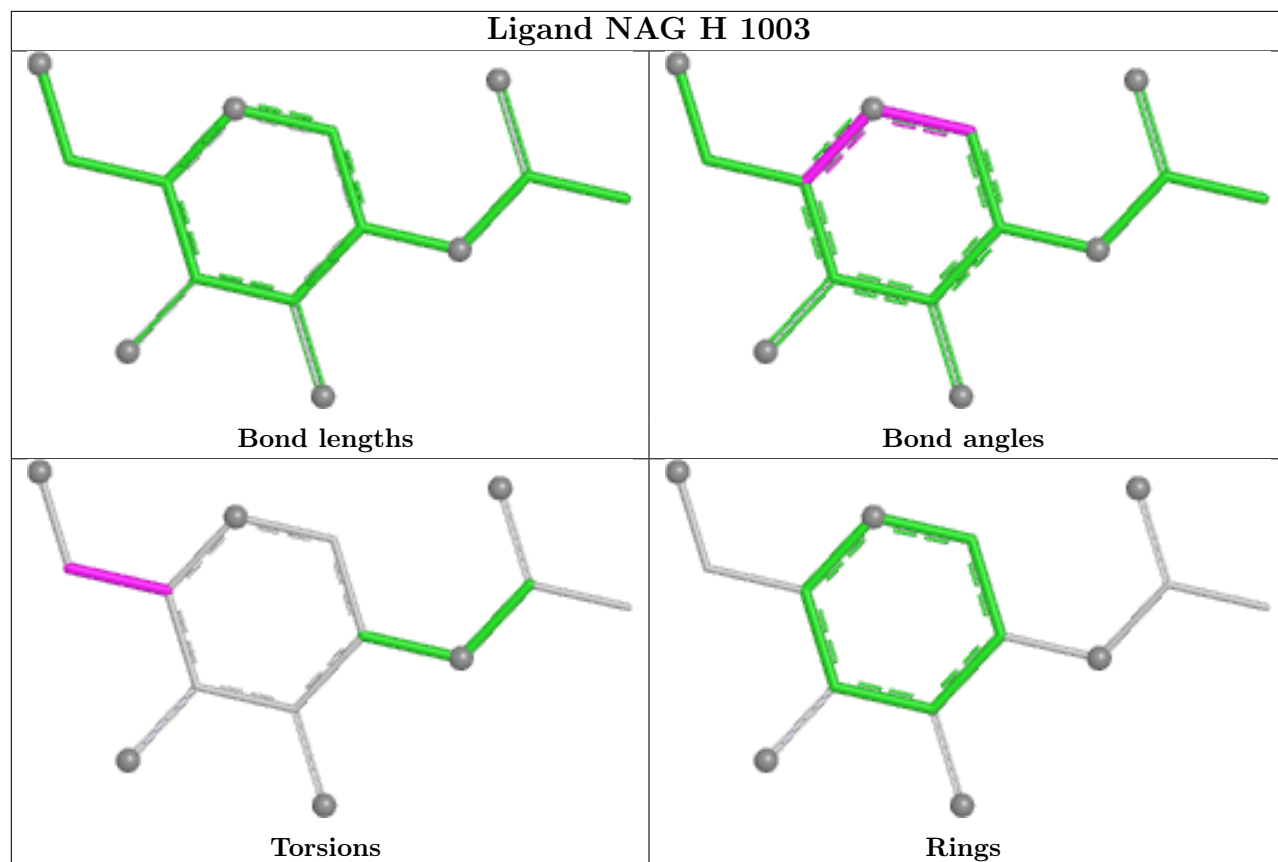




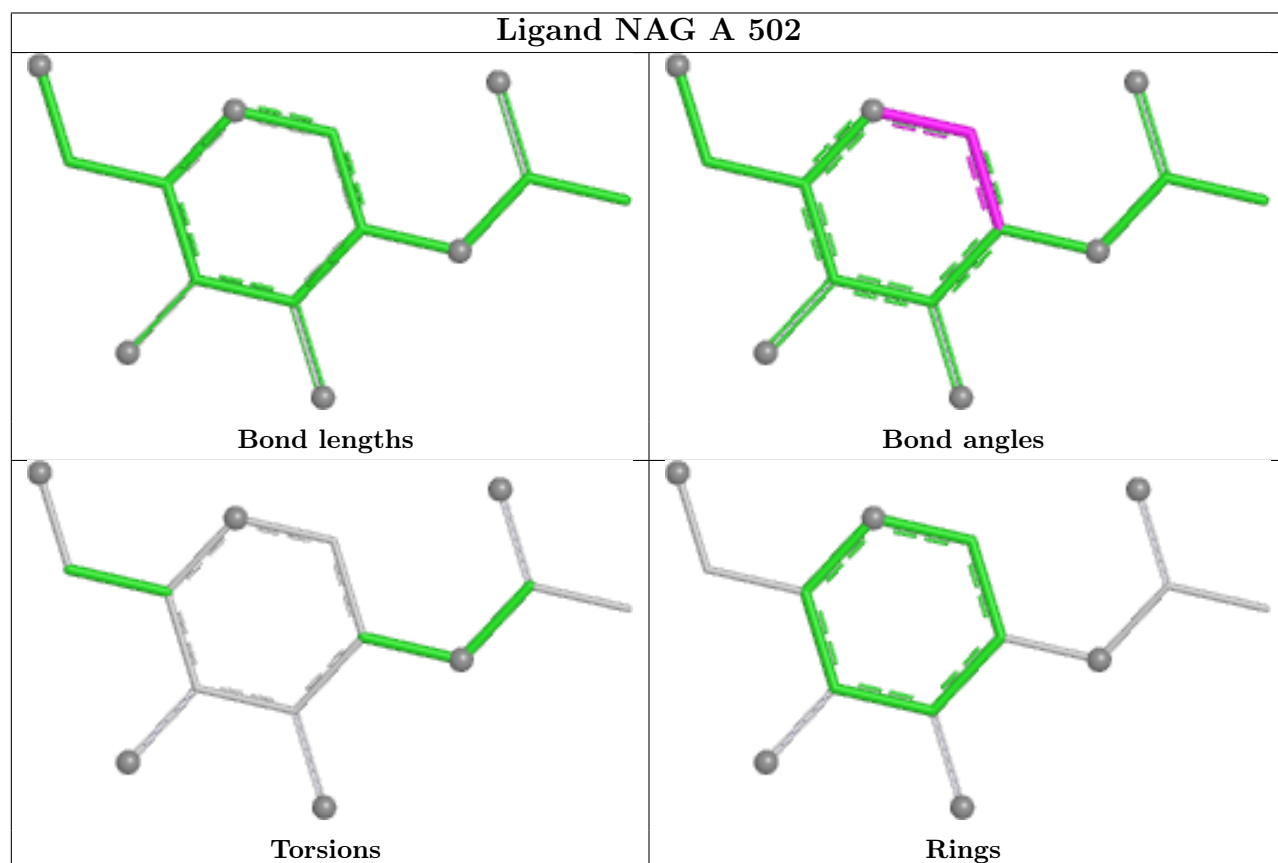


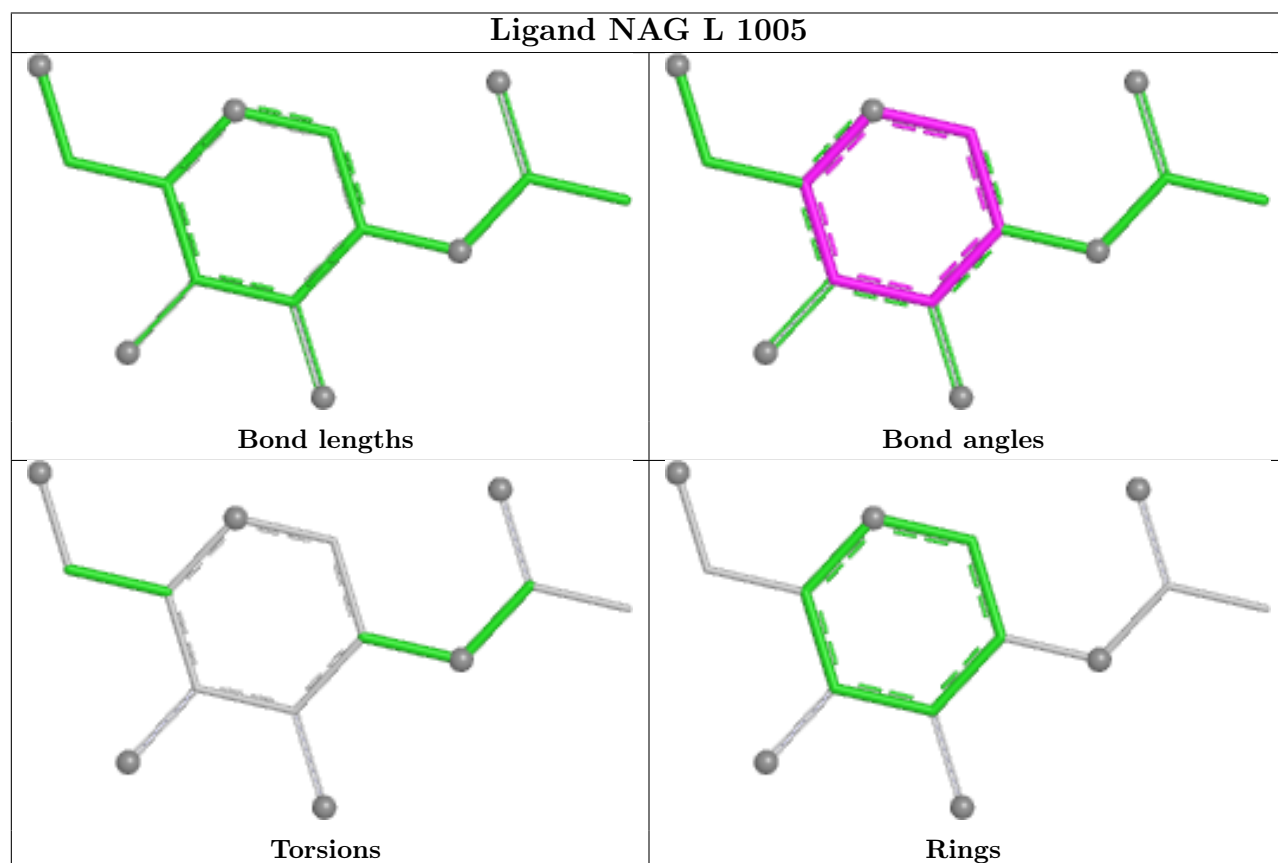
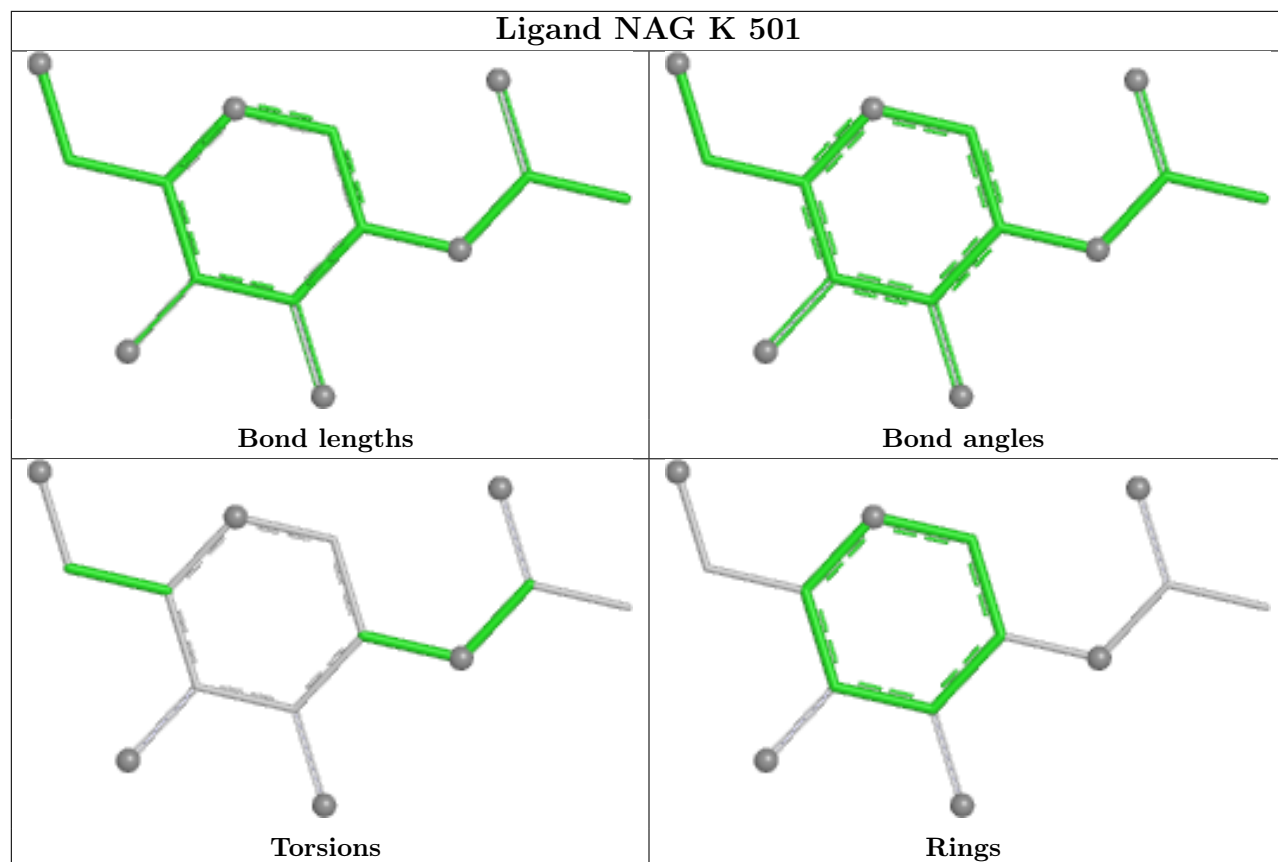


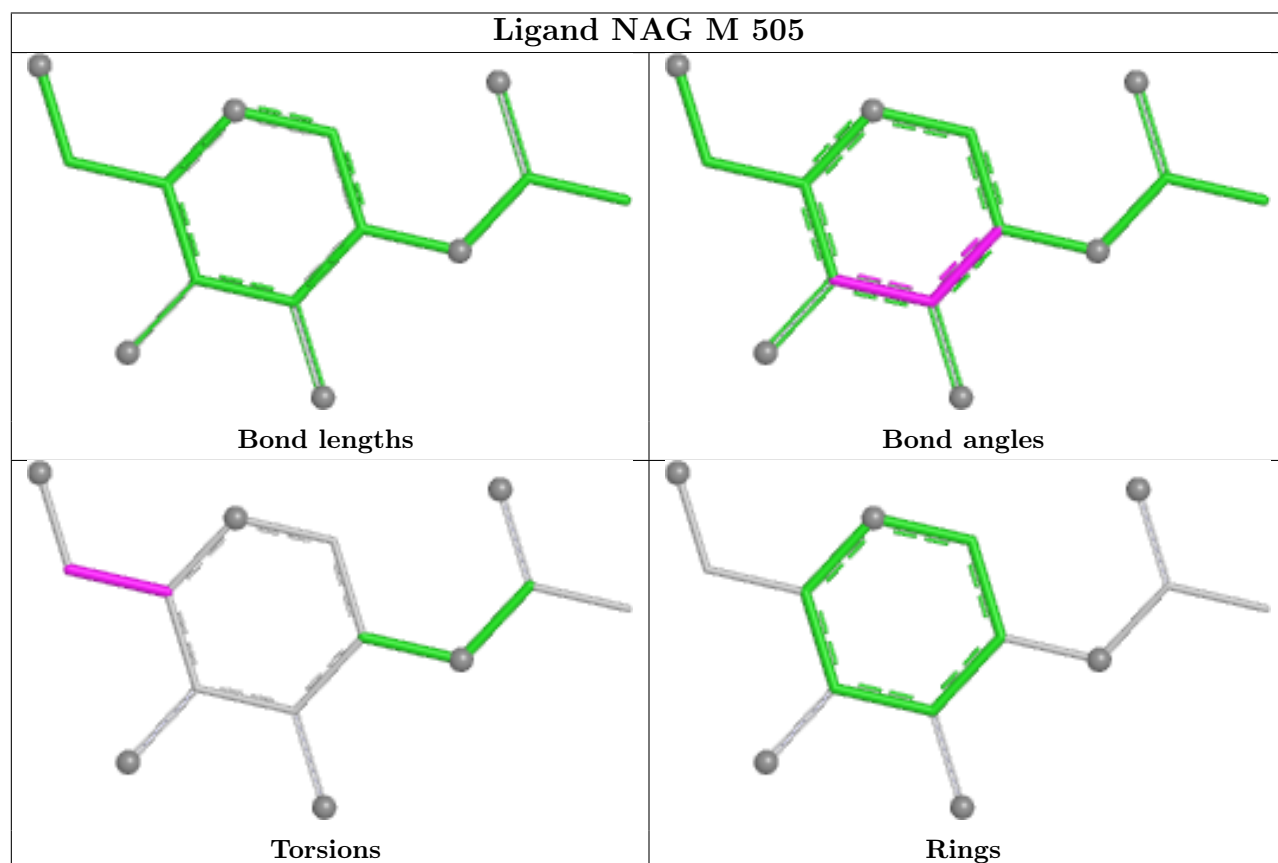
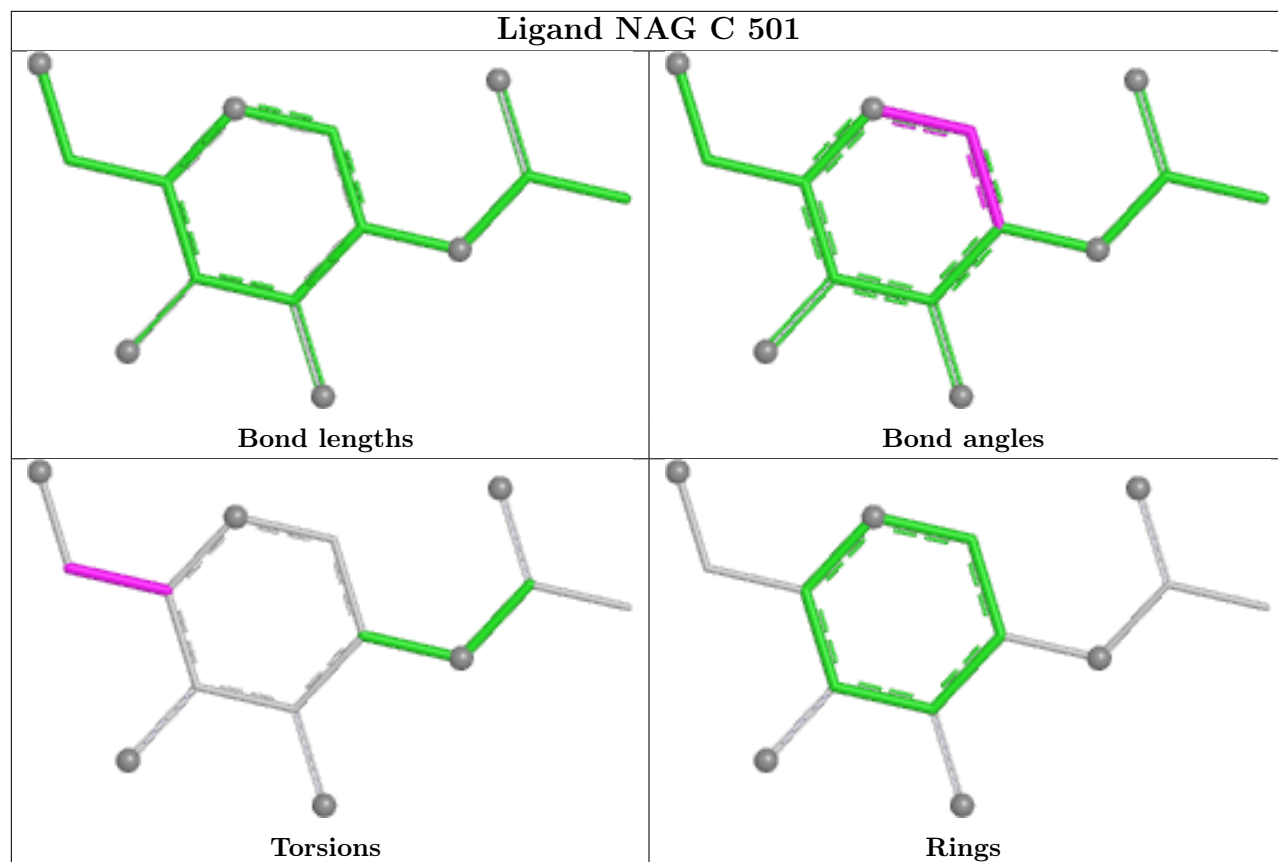
Ligand NAG H 1003



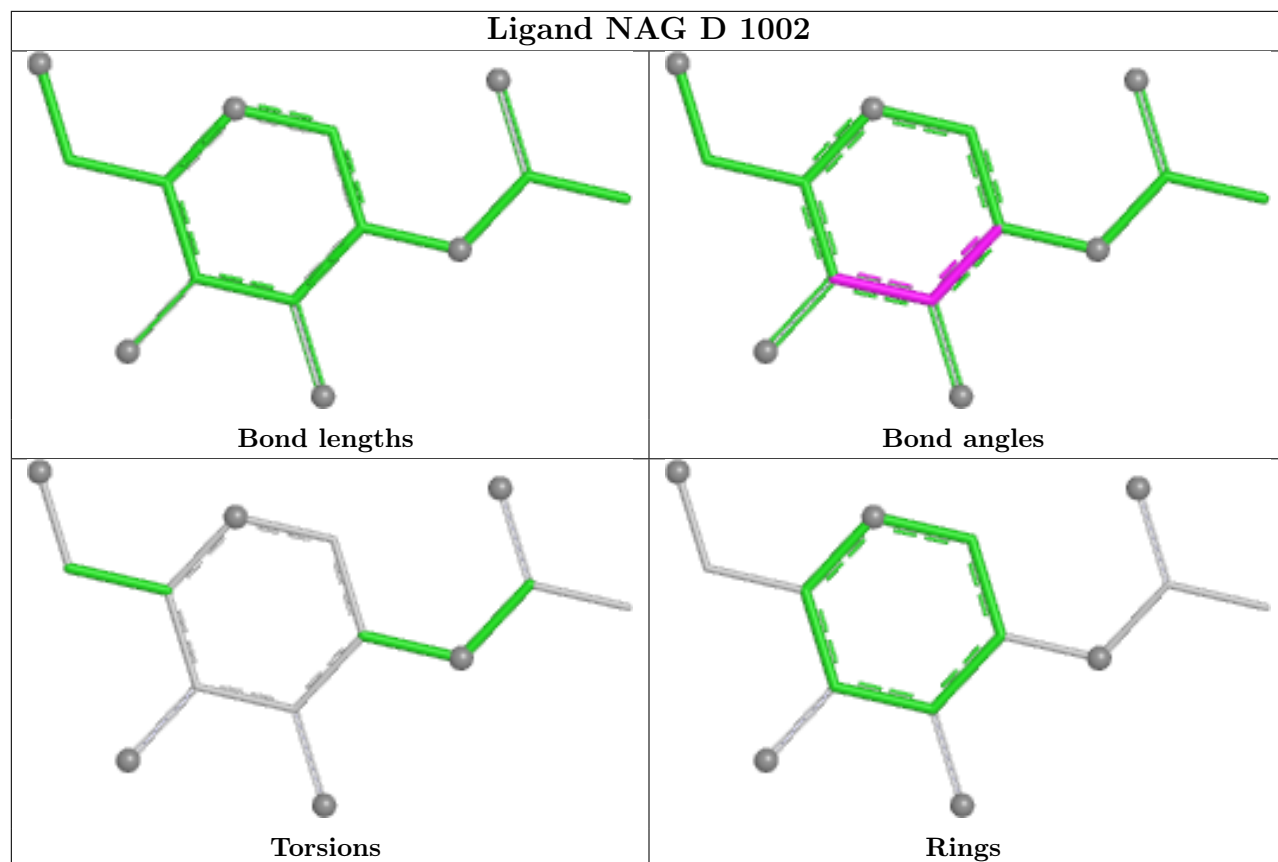
Ligand NAG A 502



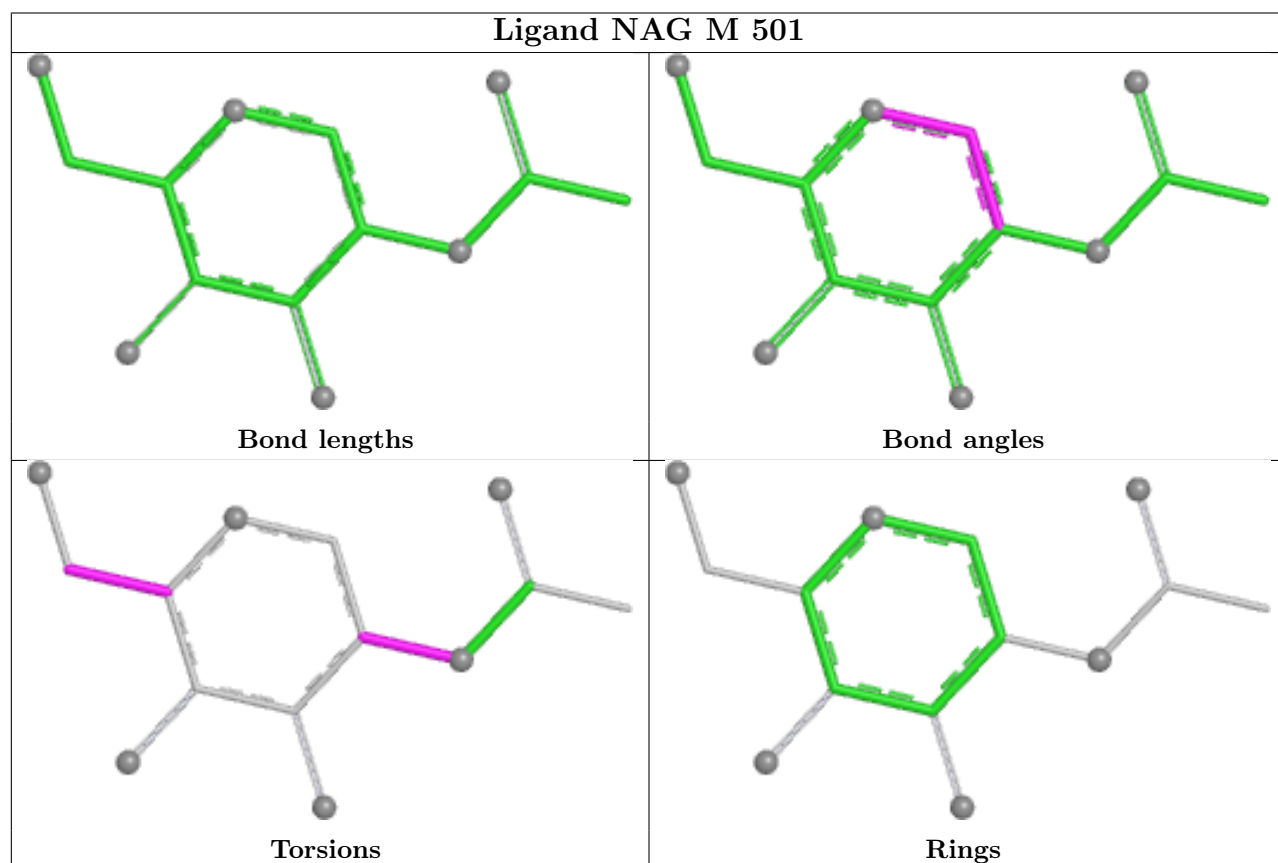


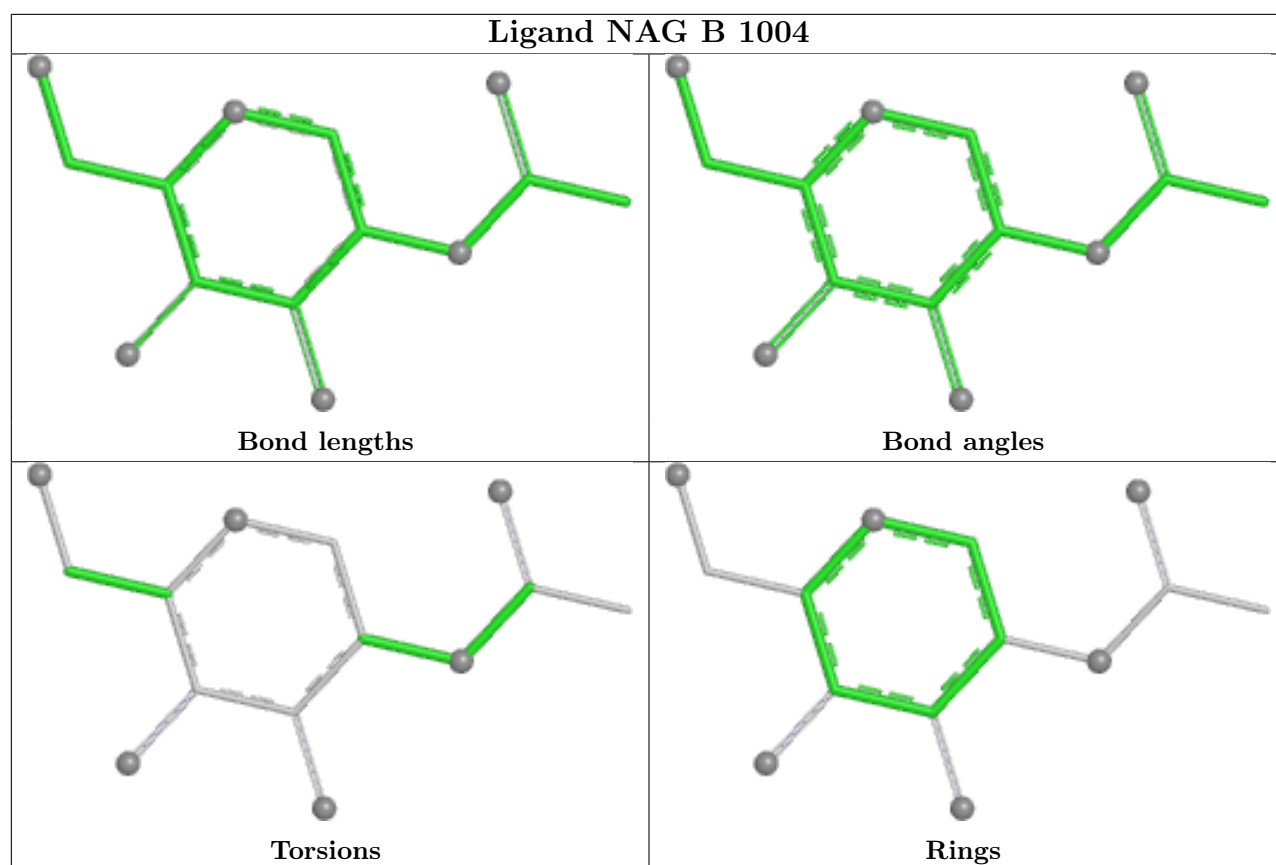


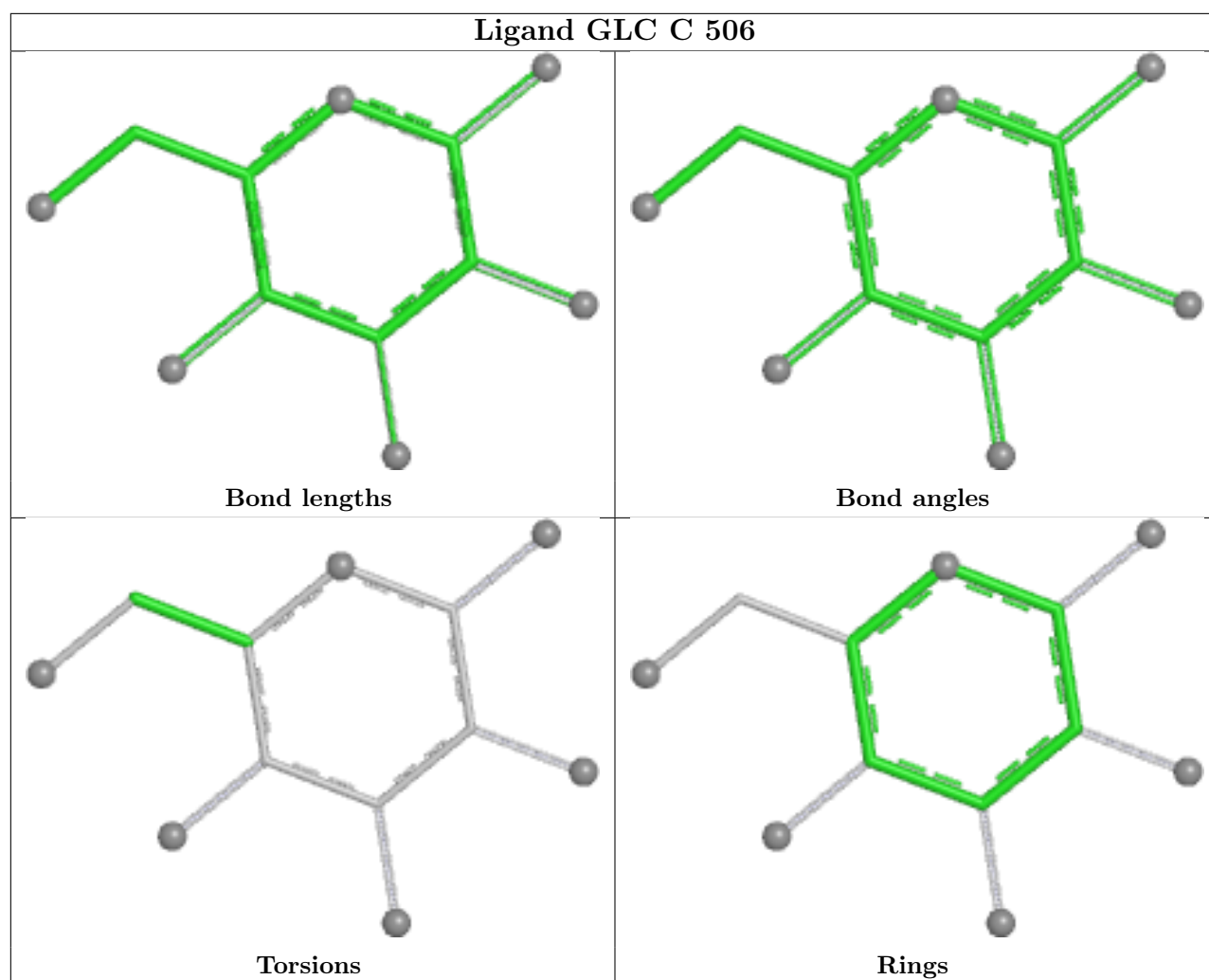
Ligand NAG D 1002



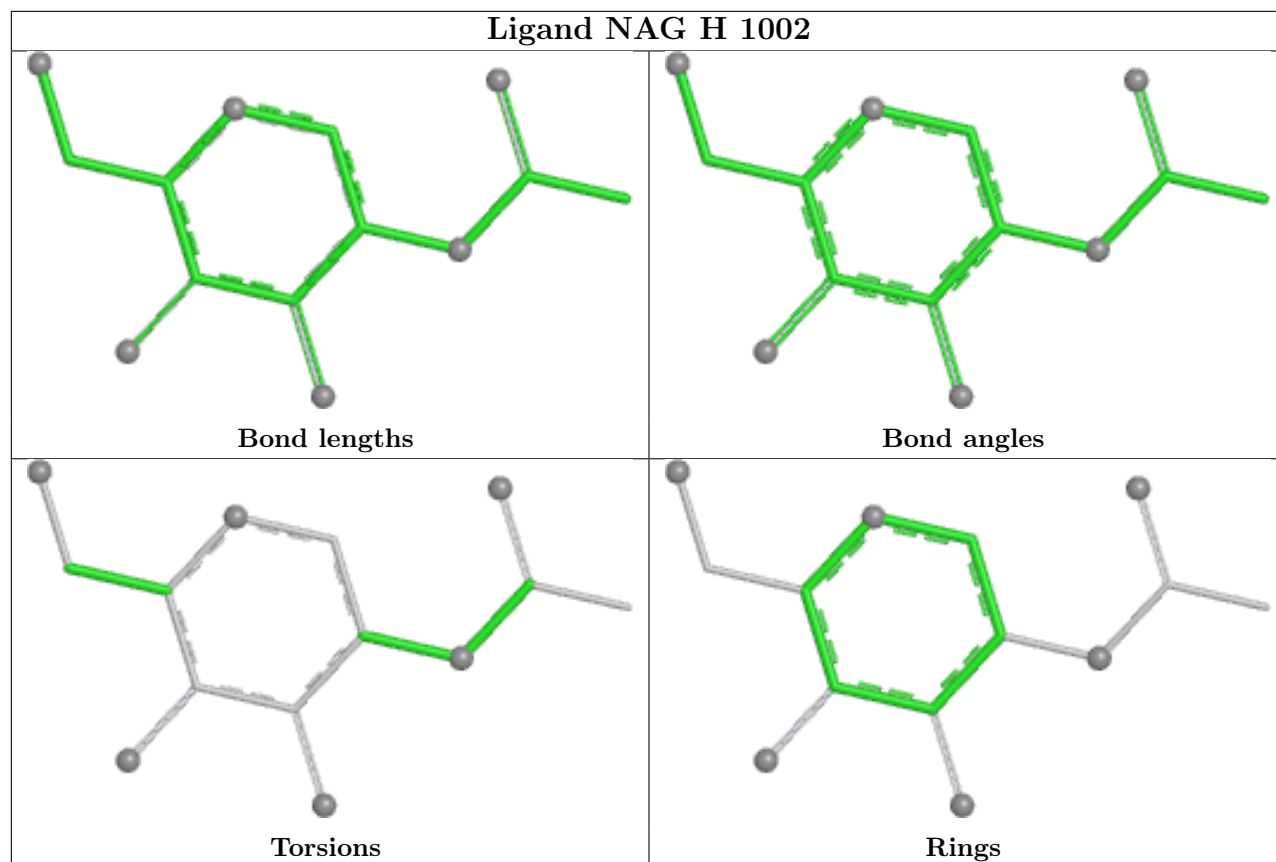
Ligand NAG M 501



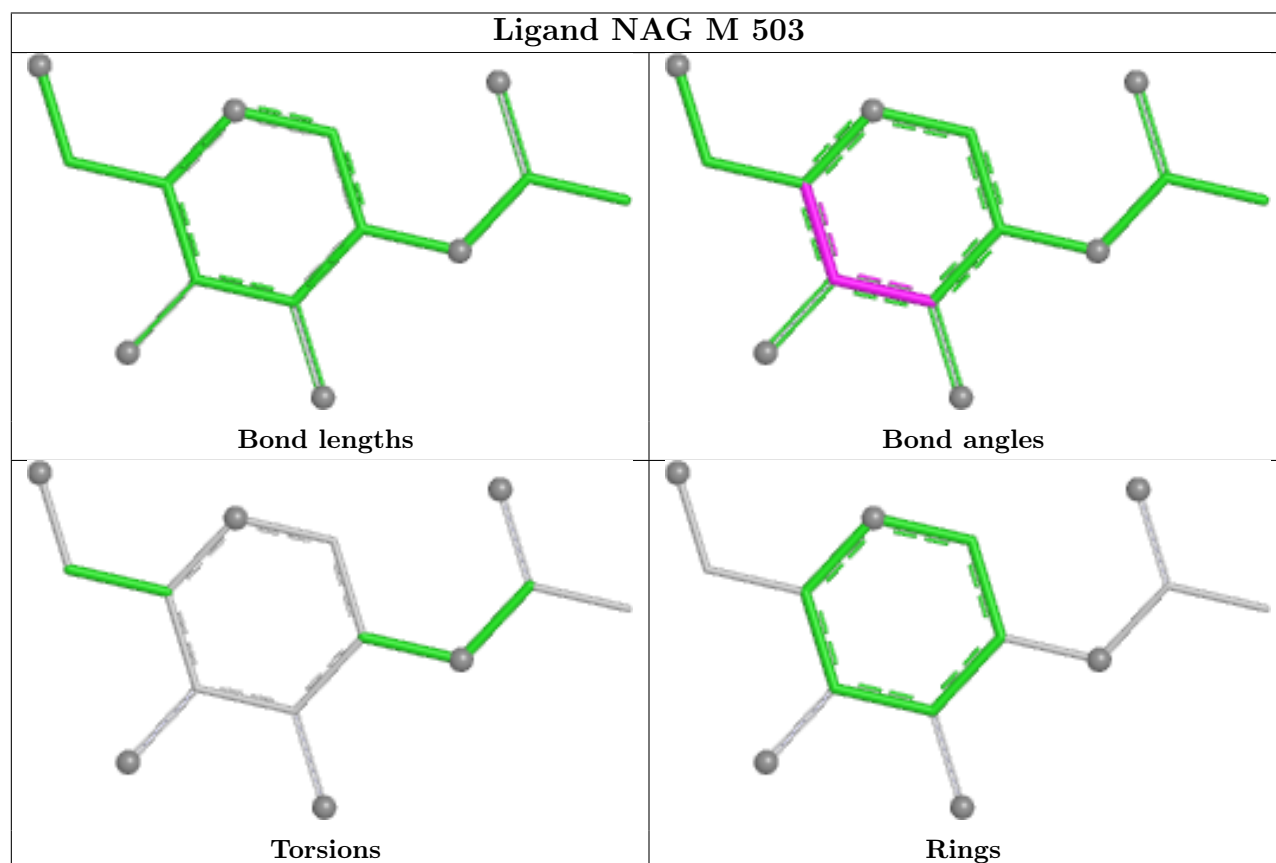


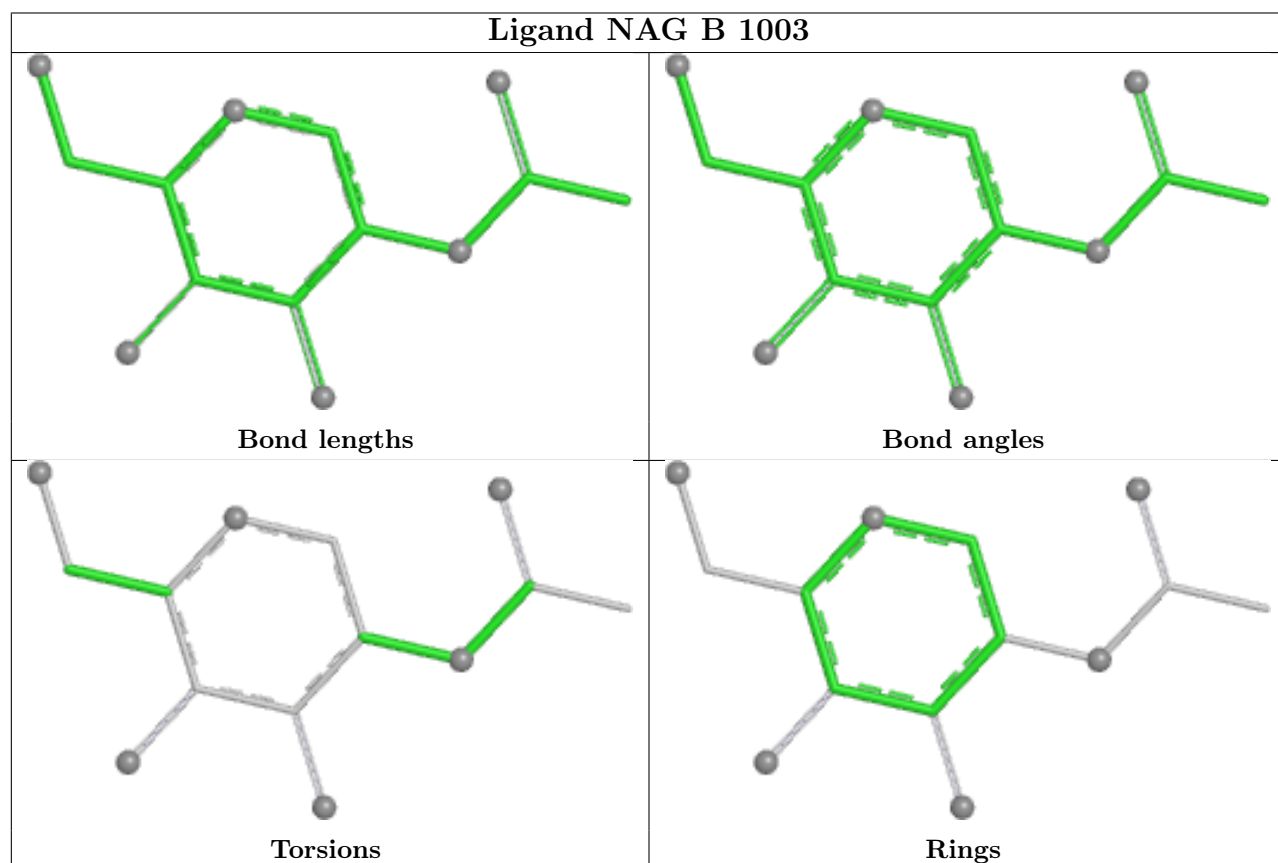
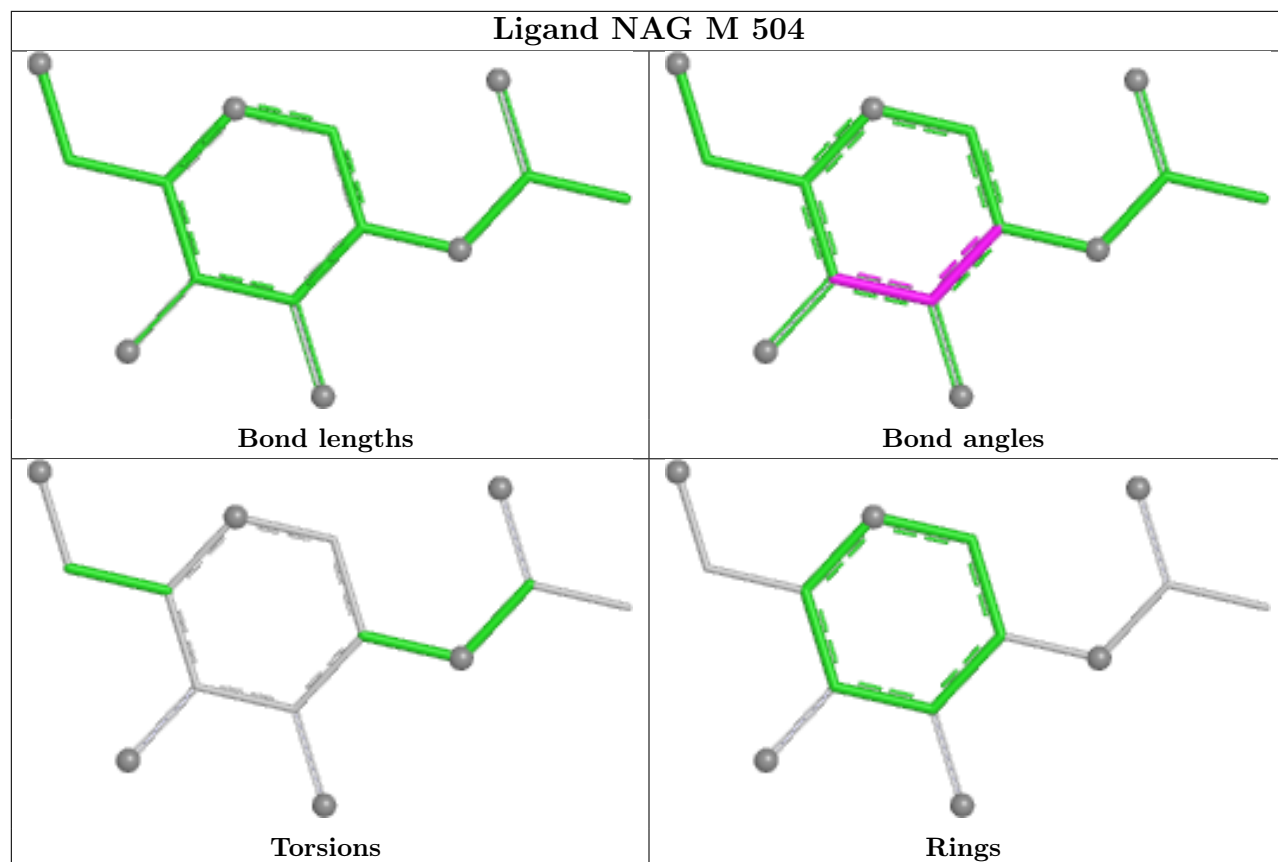


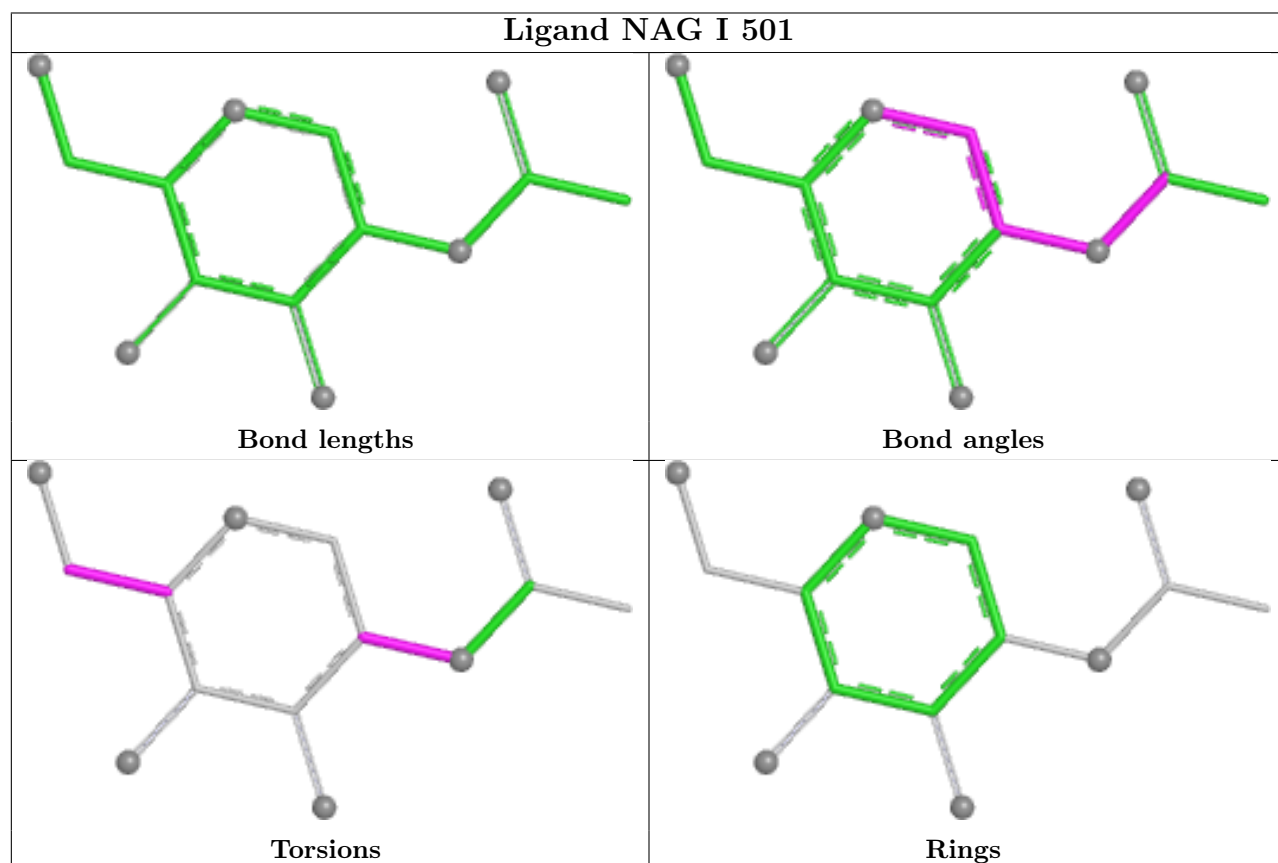
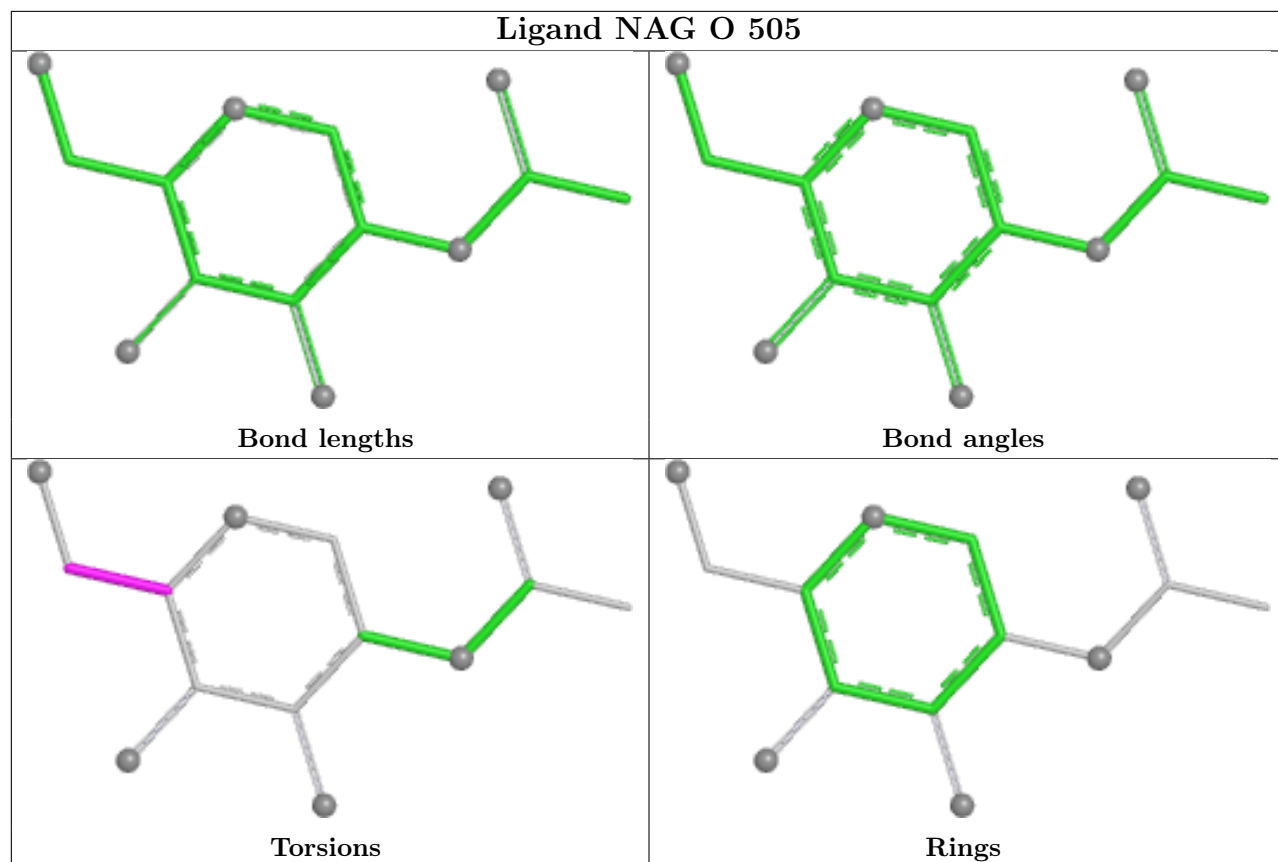
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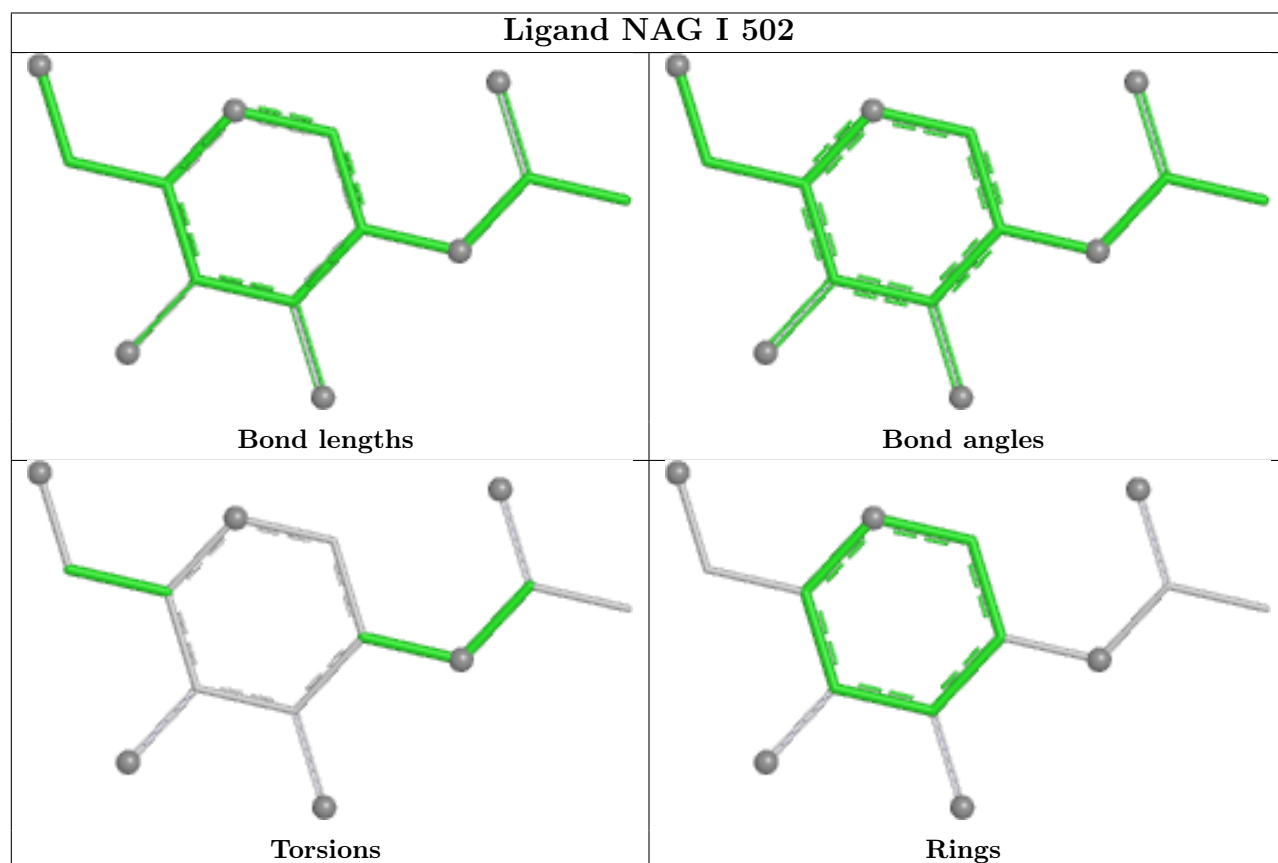
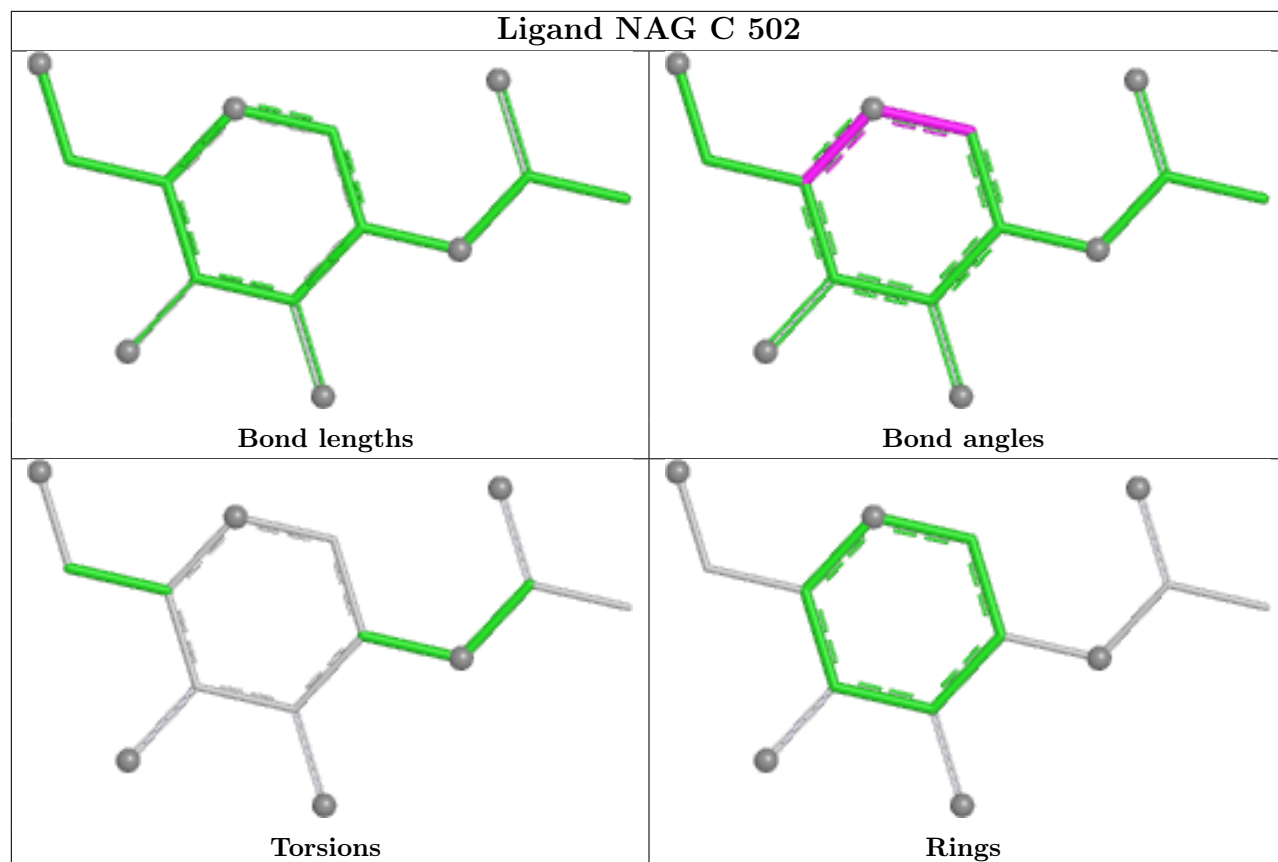


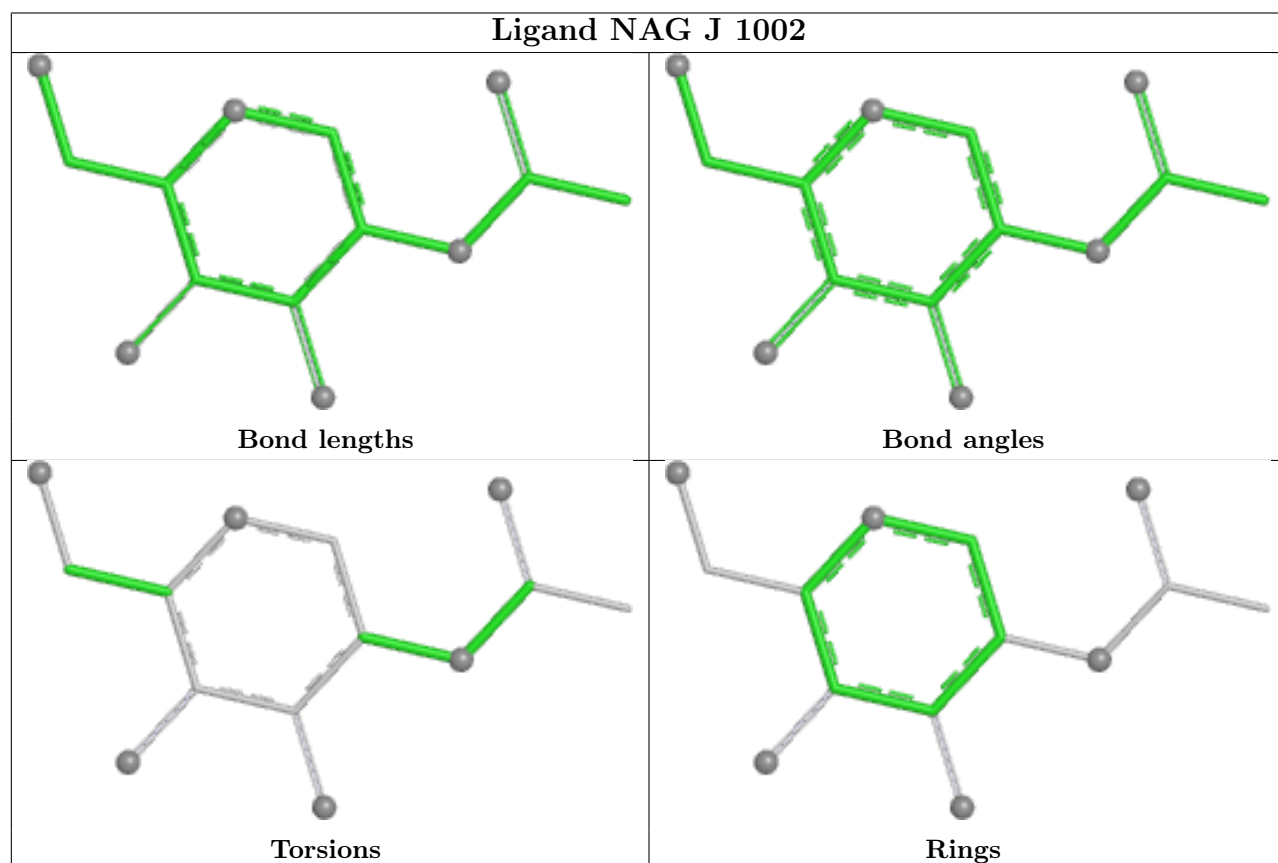
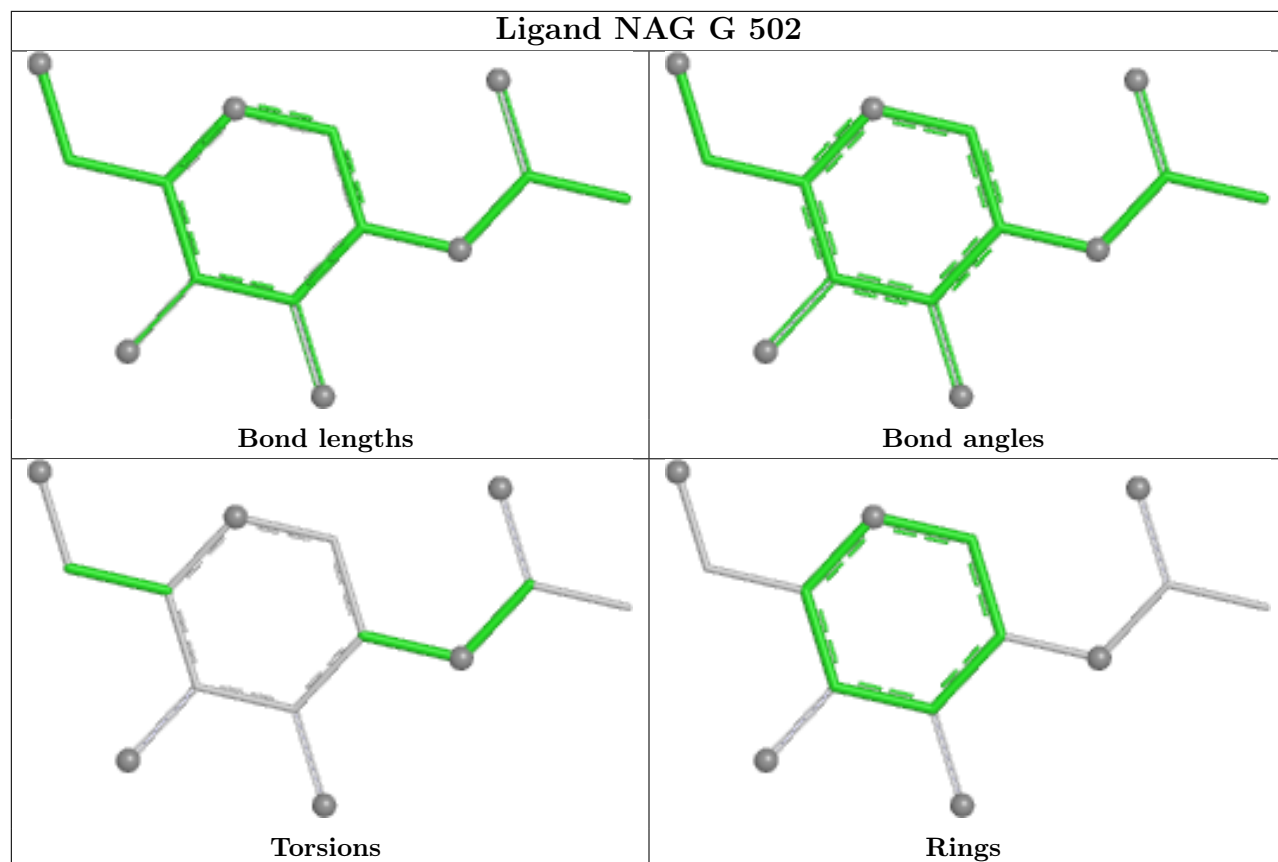
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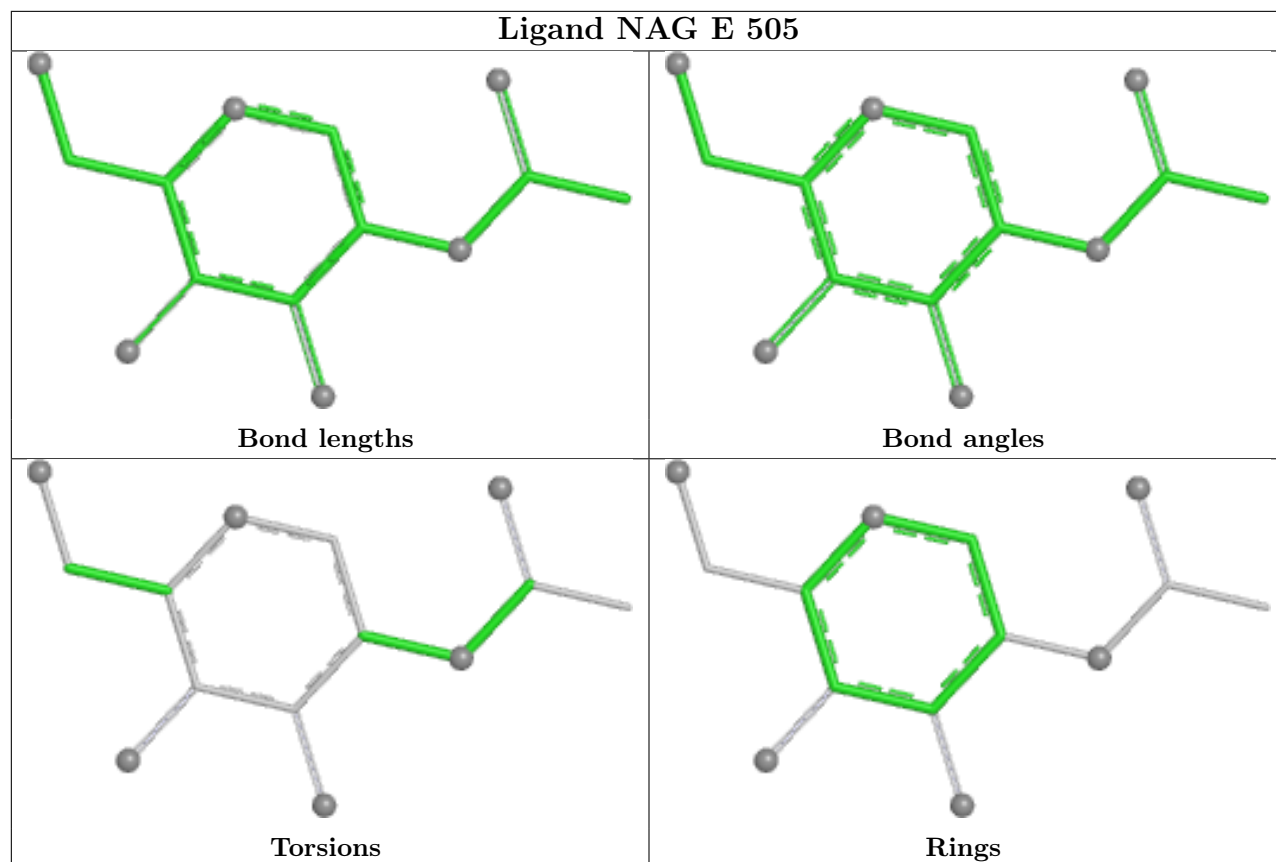












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.03	0 100 100	22, 32, 42, 72	0
1	C	465/548 (84%)	-0.95	0 100 100	25, 36, 49, 65	0
1	E	465/548 (84%)	-0.99	0 100 100	24, 34, 46, 70	0
1	G	465/548 (84%)	-0.99	0 100 100	24, 34, 46, 66	0
1	I	465/548 (84%)	-1.02	0 100 100	23, 33, 46, 65	0
1	K	465/548 (84%)	-1.02	0 100 100	24, 34, 45, 64	0
1	M	465/548 (84%)	-1.04	0 100 100	22, 32, 42, 68	0
1	O	465/548 (84%)	-0.95	0 100 100	25, 36, 49, 70	0
2	B	436/445 (97%)	-1.00	0 100 100	22, 31, 51, 83	0
2	D	436/445 (97%)	-0.94	0 100 100	25, 34, 55, 91	0
2	F	436/445 (97%)	-0.96	0 100 100	24, 32, 52, 85	0
2	H	436/445 (97%)	-0.95	0 100 100	25, 34, 56, 85	0
2	J	436/445 (97%)	-0.90	0 100 100	22, 34, 58, 91	0
2	L	436/445 (97%)	-0.89	0 100 100	25, 35, 59, 83	0
2	N	436/445 (97%)	-0.95	0 100 100	22, 33, 53, 83	0
2	P	436/445 (97%)	-0.85	0 100 100	26, 37, 61, 90	0
All	All	7208/7944 (90%)	-0.97	0 100 100	22, 34, 51, 91	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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	T	3	11/12	0.92	0.09	59,60,62,64	0
5	BMA	X	3	11/12	0.92	0.09	55,58,60,64	0
4	NAG	V	2	14/15	0.95	0.07	50,56,61,62	0
4	NAG	R	2	14/15	0.96	0.06	45,48,49,52	0
5	NAG	X	2	14/15	0.96	0.07	37,45,49,53	0
4	NAG	Z	2	14/15	0.96	0.07	51,56,60,60	0
3	GLC	W	2	11/12	0.97	0.05	43,45,46,47	0
3	GLC	U	2	11/12	0.97	0.05	39,43,47,48	0
5	NAG	T	2	14/15	0.97	0.06	38,45,49,55	0
4	NAG	Z	1	14/15	0.98	0.04	39,40,44,47	0
3	GLC	a	1	12/12	-	-	36,37,38,39	0
3	GLC	a	2	11/12	-	-	42,43,44,44	0
3	GLC	c	1	12/12	-	-	37,38,39,40	0
3	GLC	c	2	11/12	-	-	37,39,40,40	0
3	GLC	e	1	12/12	-	-	38,40,40,41	0
3	GLC	e	2	11/12	-	-	41,43,44,44	0
3	GLC	g	1	12/12	-	-	30,33,34,36	0
3	GLC	g	2	11/12	-	-	33,34,35,36	0
3	GLC	i	1	12/12	-	-	40,42,43,44	0
3	GLC	i	2	11/12	-	-	43,44,45,46	0
3	GLC	k	1	12/12	-	-	33,35,37,37	0
3	GLC	k	2	11/12	-	-	37,39,40,40	0
3	GLC	m	1	12/12	-	-	38,43,44,44	0
3	GLC	m	2	11/12	-	-	41,43,44,44	0
3	GLC	o	1	12/12	-	-	28,31,32,34	0
3	GLC	o	2	11/12	-	-	37,37,38,39	0
3	GLC	q	1	12/12	-	-	37,40,42,43	0
3	GLC	q	2	11/12	-	-	39,41,41,42	0
3	GLC	s	1	12/12	-	-	32,36,37,38	0
3	GLC	s	2	11/12	-	-	41,43,45,45	0
3	GLC	u	1	12/12	-	-	43,46,47,49	0
3	GLC	u	2	11/12	-	-	48,49,50,51	0
3	GLC	S	2	11/12	0.98	0.05	36,38,39,40	0
3	GLC	Y	2	11/12	0.98	0.04	34,37,38,38	0
3	GLC	U	1	12/12	0.98	0.05	39,40,42,43	0
5	NAG	X	1	14/15	0.98	0.04	33,36,39,39	0
4	NAG	V	1	14/15	0.98	0.05	36,42,45,49	0

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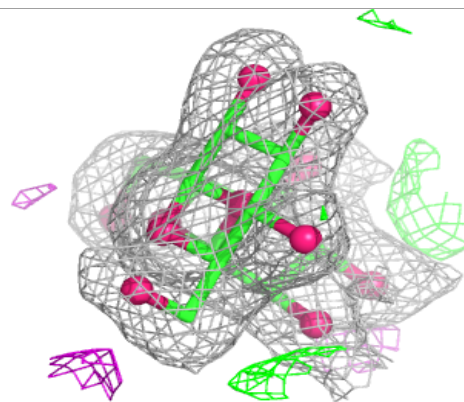
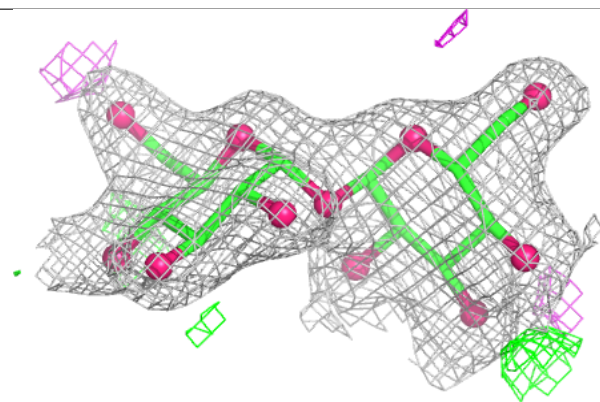
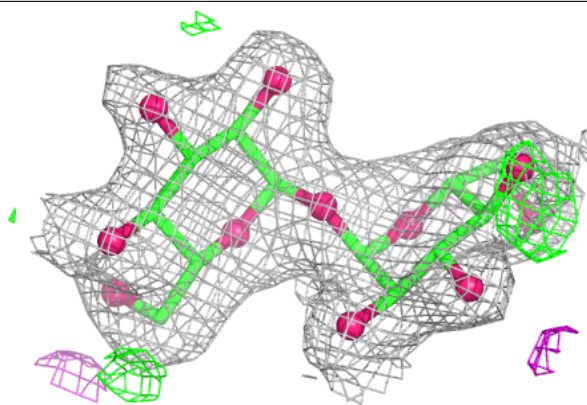
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	Q	2	11/12	0.98	0.04	33,34,36,37	0
4	NAG	d	1	14/15	-	-	39,40,46,47	0
4	NAG	d	2	14/15	-	-	51,53,55,56	0
4	NAG	h	1	14/15	-	-	37,40,42,44	0
4	NAG	h	2	14/15	-	-	46,50,51,54	0
4	NAG	l	1	14/15	-	-	36,38,40,42	0
4	NAG	l	2	14/15	-	-	48,50,54,55	0
4	NAG	p	1	14/15	-	-	41,43,45,48	0
4	NAG	p	2	14/15	-	-	52,55,58,59	0
4	NAG	t	1	14/15	-	-	42,49,54,54	0
4	NAG	t	2	14/15	-	-	51,59,62,64	0
5	NAG	T	1	14/15	0.99	0.04	28,31,33,38	0
3	GLC	W	1	12/12	0.99	0.04	35,38,38,39	0
3	GLC	S	1	12/12	0.99	0.04	32,33,35,36	0
3	GLC	Y	1	12/12	0.99	0.04	32,36,36,37	0
3	GLC	Q	1	12/12	0.99	0.04	32,35,36,38	0
4	NAG	R	1	14/15	0.99	0.04	35,36,39,41	0
5	NAG	b	1	14/15	-	-	28,30,33,36	0
5	NAG	b	2	14/15	-	-	38,44,49,56	0
5	BMA	b	3	11/12	-	-	62,64,65,66	0
5	NAG	f	1	14/15	-	-	31,34,35,39	0
5	NAG	f	2	14/15	-	-	42,45,49,54	0
5	BMA	f	3	11/12	-	-	56,61,65,65	0
5	NAG	j	1	14/15	-	-	31,36,38,41	0
5	NAG	j	2	14/15	-	-	46,49,54,59	0
5	BMA	j	3	11/12	-	-	63,66,67,68	0
5	NAG	n	1	14/15	-	-	35,38,43,44	0
5	NAG	n	2	14/15	-	-	45,50,53,56	0
5	BMA	n	3	11/12	-	-	61,63,65,68	0
5	NAG	r	1	14/15	-	-	32,36,38,41	0
5	NAG	r	2	14/15	-	-	42,47,52,58	0
5	BMA	r	3	11/12	-	-	60,63,64,65	0
5	NAG	v	1	14/15	-	-	31,37,39,42	0
5	NAG	v	2	14/15	-	-	41,48,53,59	0
5	BMA	v	3	11/12	-	-	62,65,68,70	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.

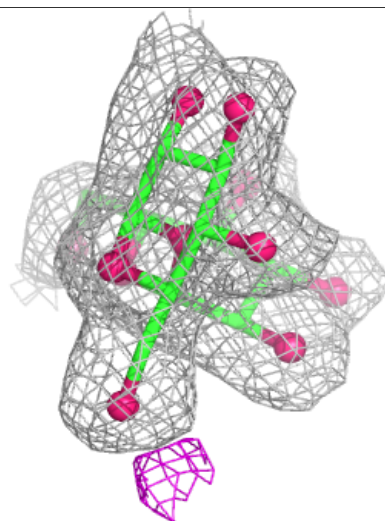
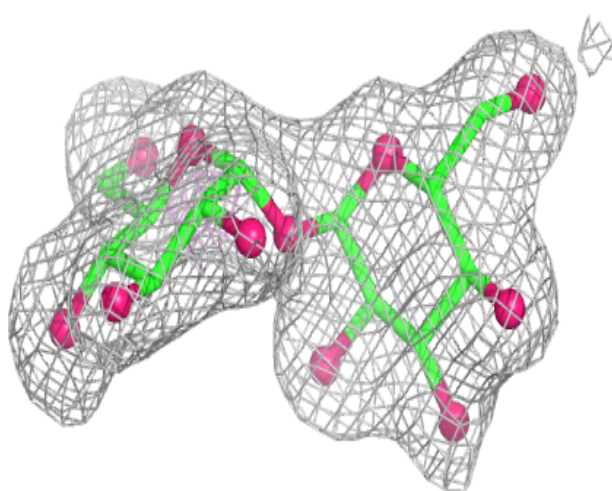
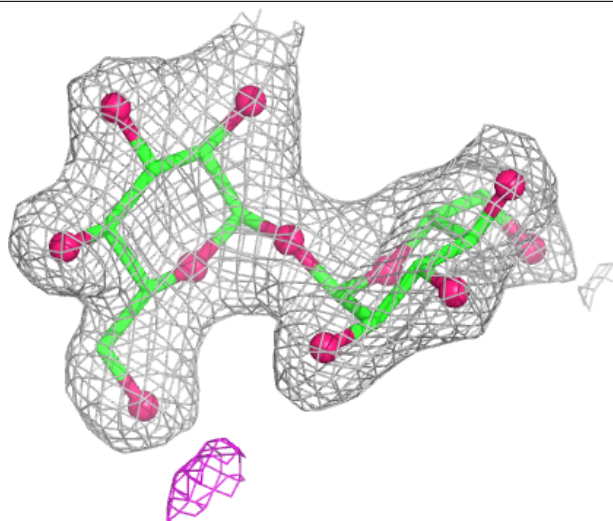
Electron density around Chain Q:

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



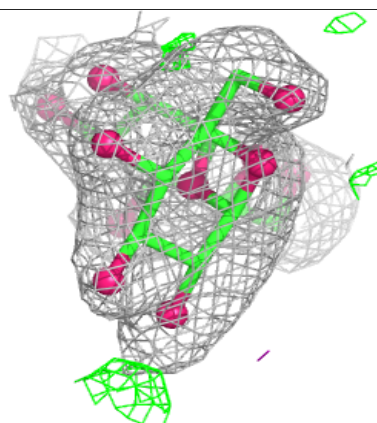
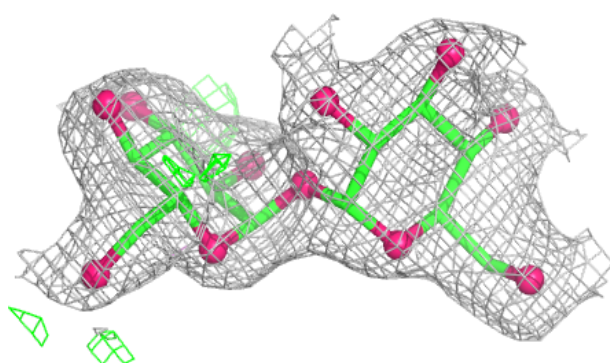
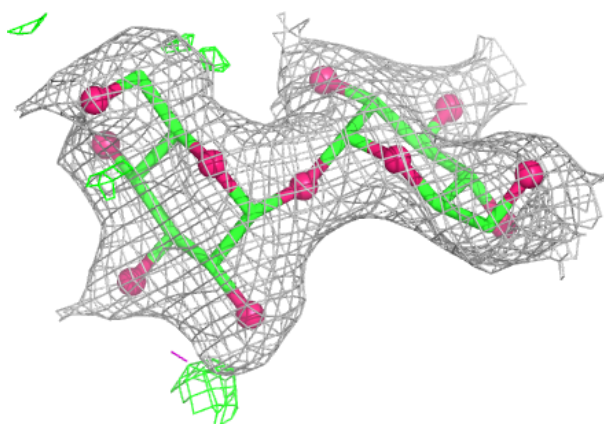
Electron density around Chain S:

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

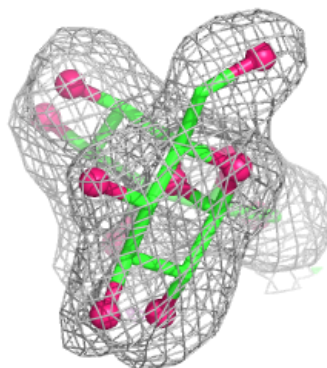
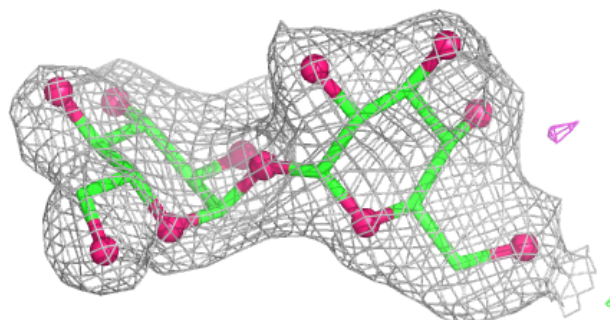
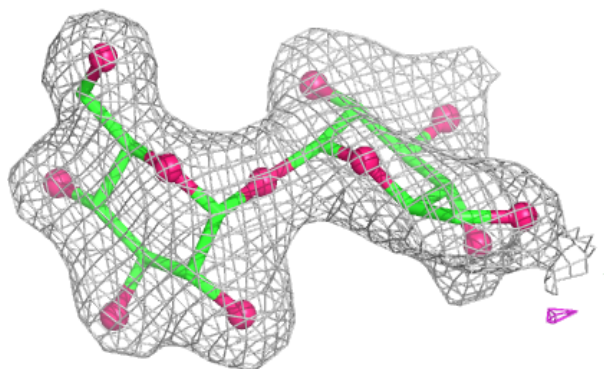


Electron density around Chain U:

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

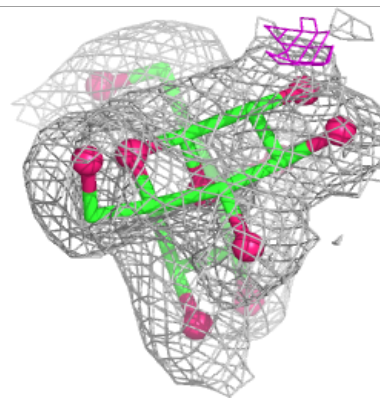
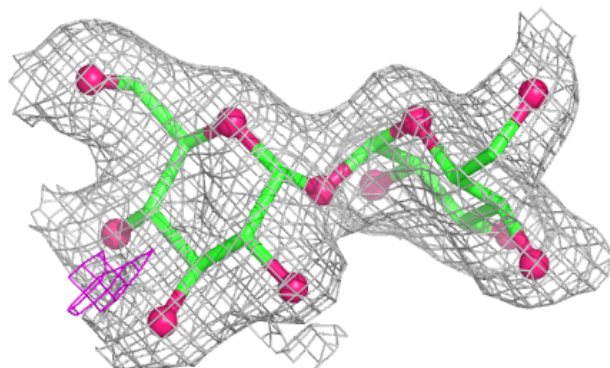
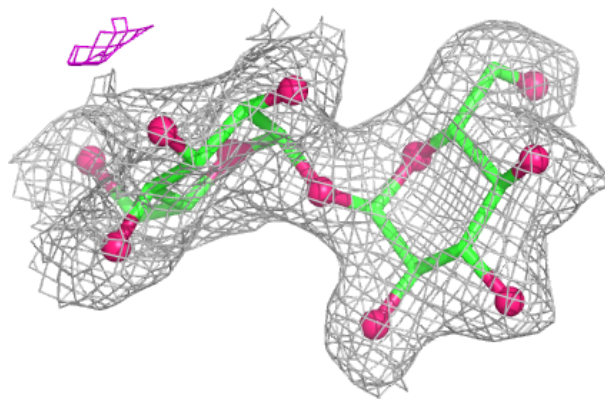
**Electron density around Chain W:**

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



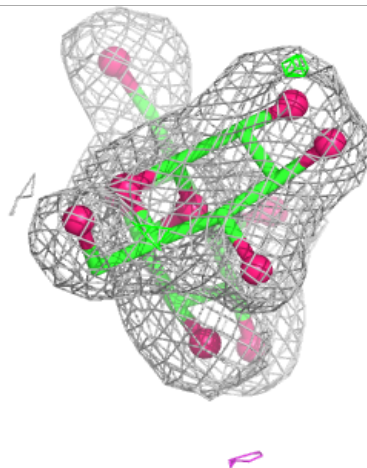
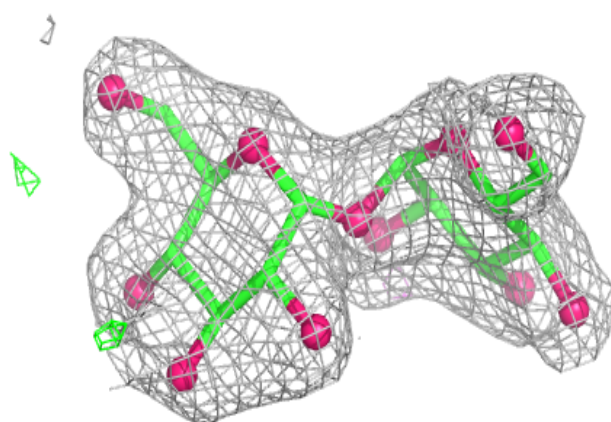
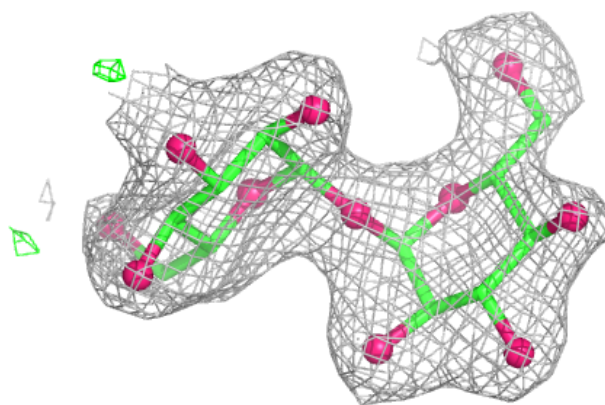
Electron density around Chain Y:

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



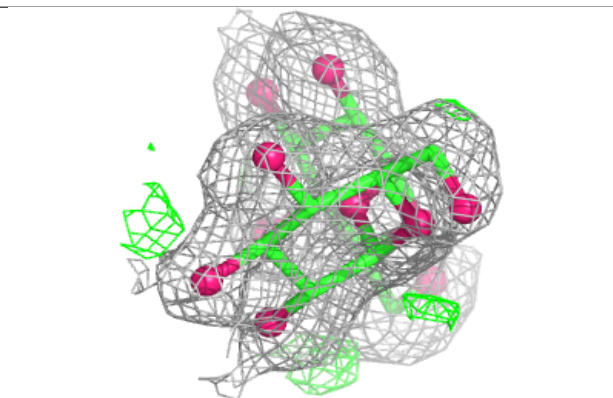
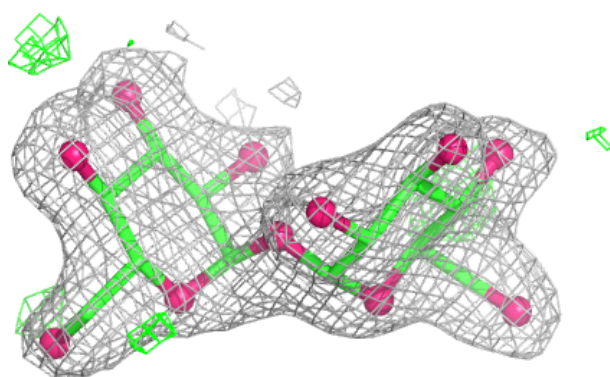
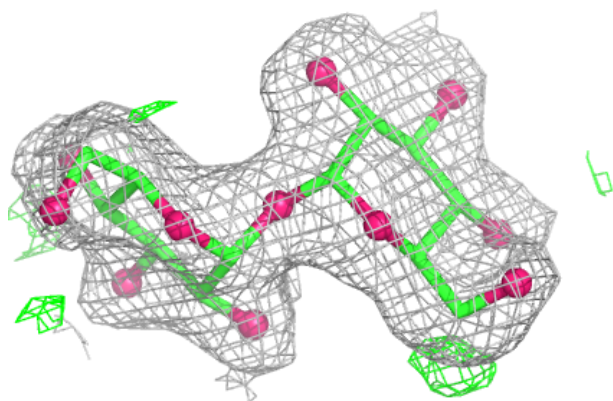
Electron density around Chain a:

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

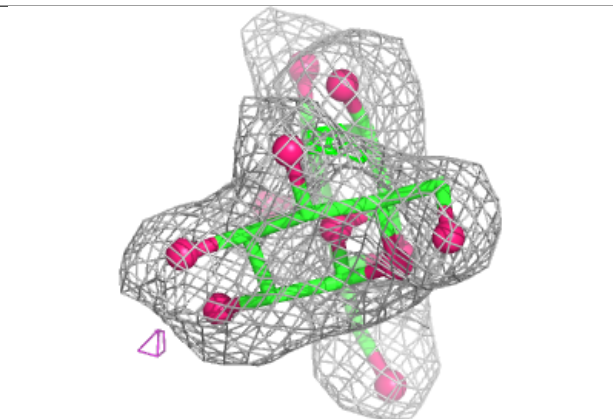
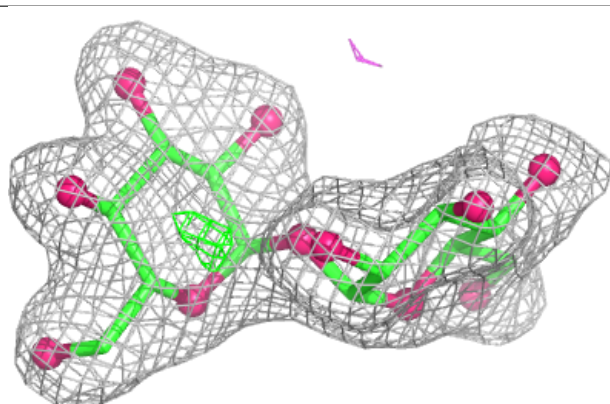
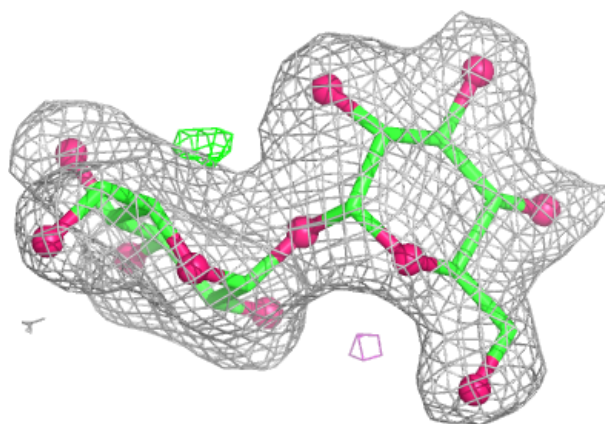


Electron density around Chain c:

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

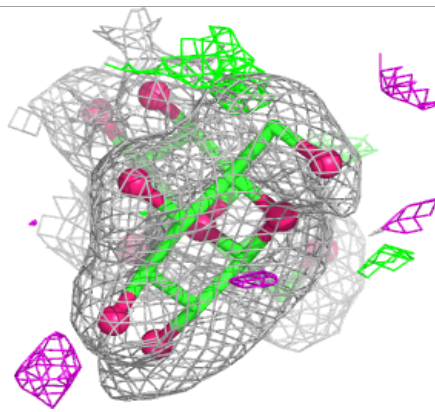
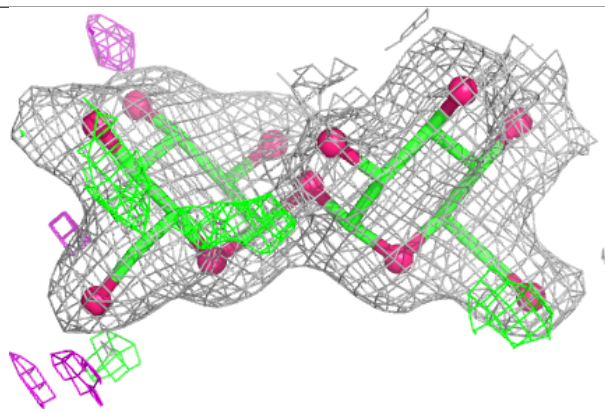
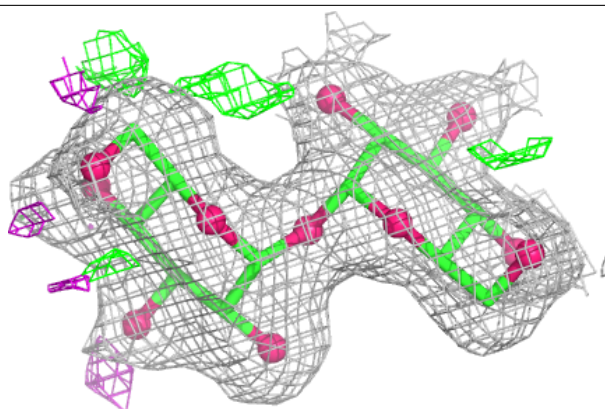
**Electron density around Chain e:**

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



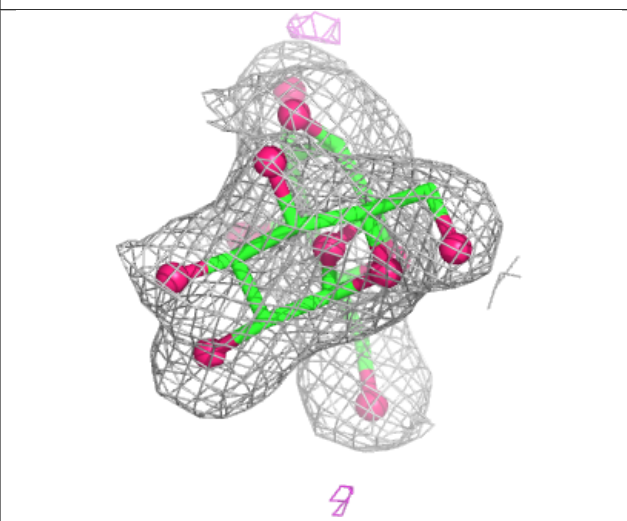
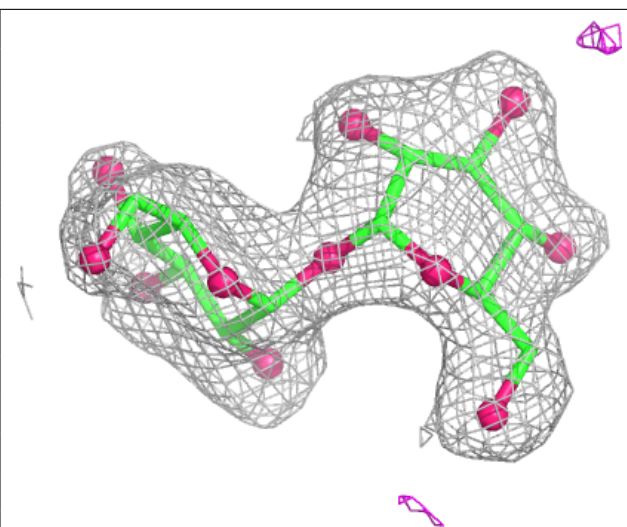
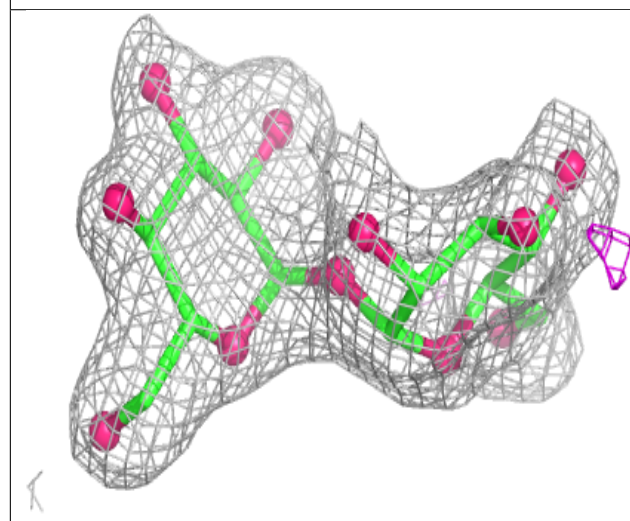
Electron density around Chain g:

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



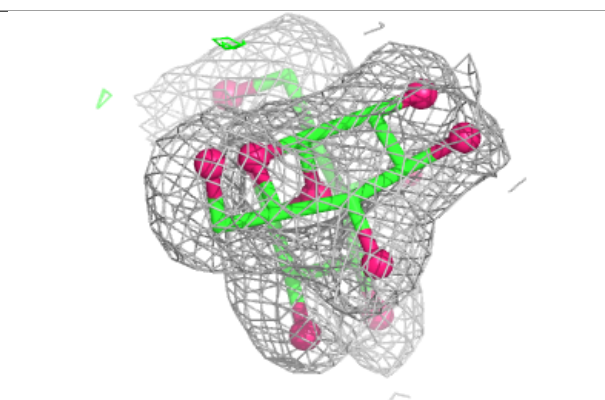
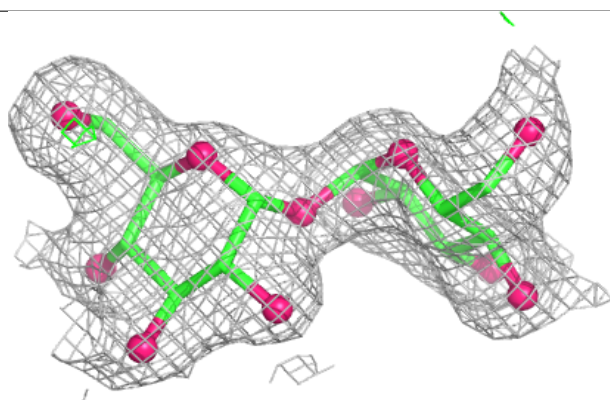
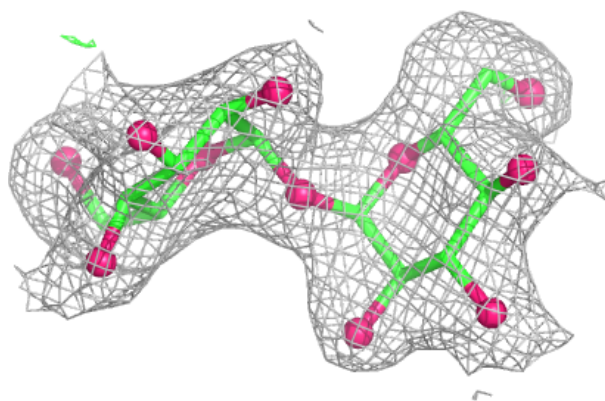
Electron density around Chain i:

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and green (positive)

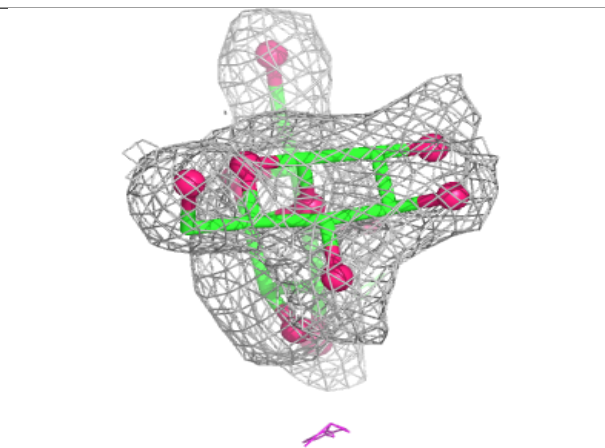
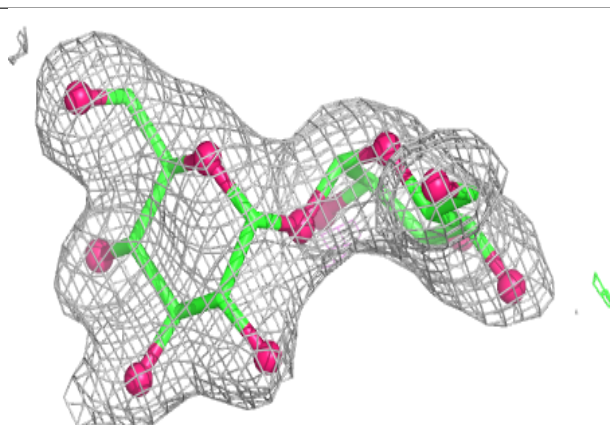
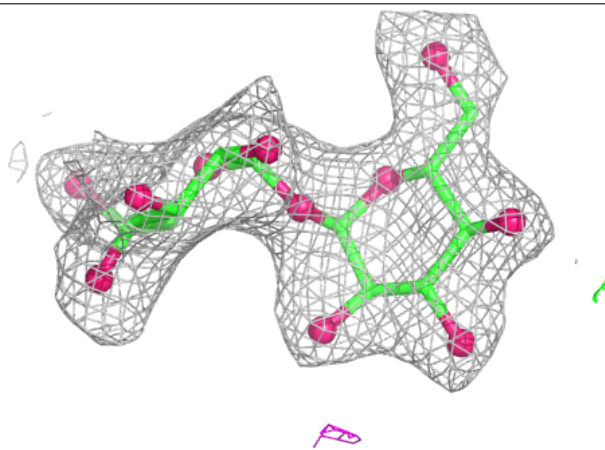


Electron density around Chain k:

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

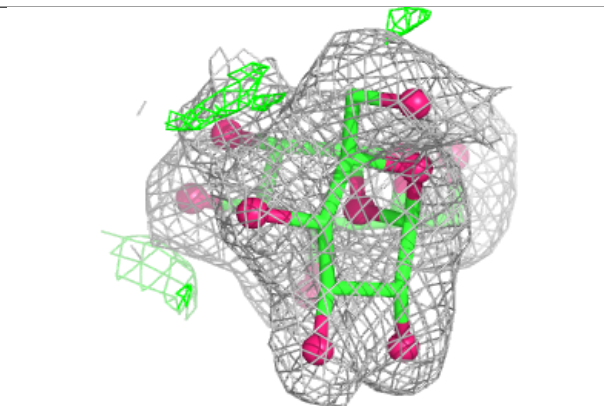
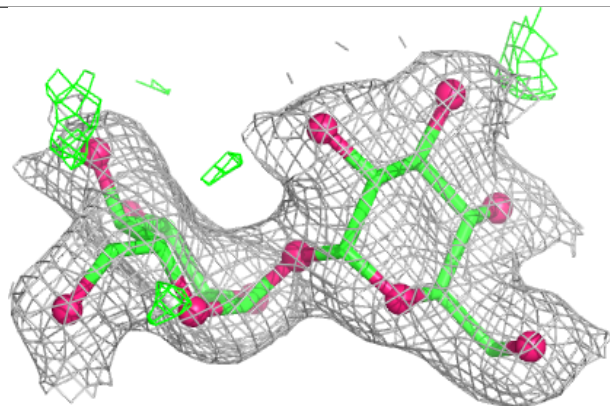
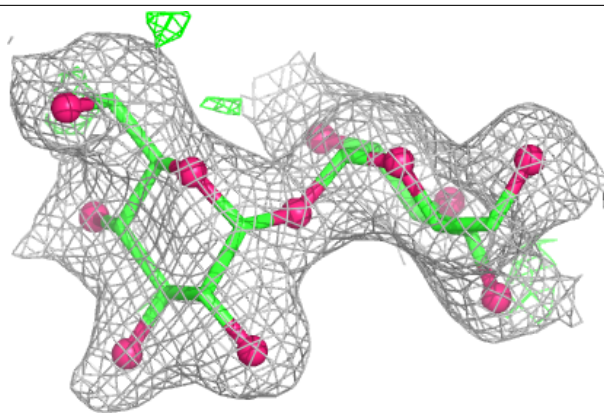
**Electron density around Chain m:**

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

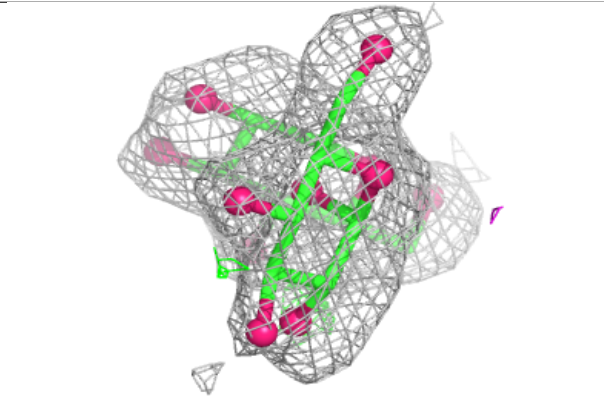
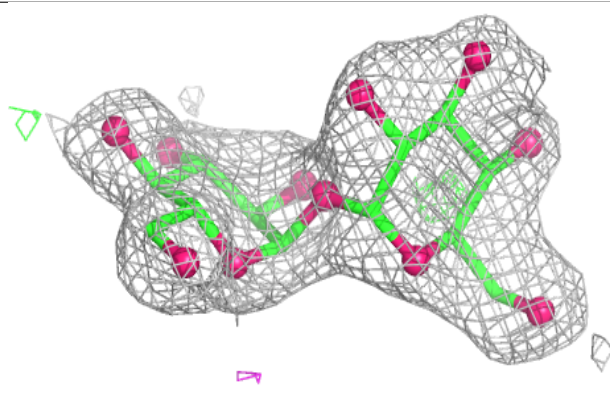
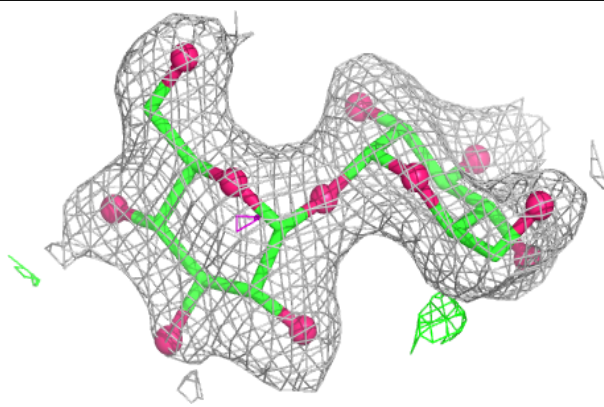


Electron density around Chain o:

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

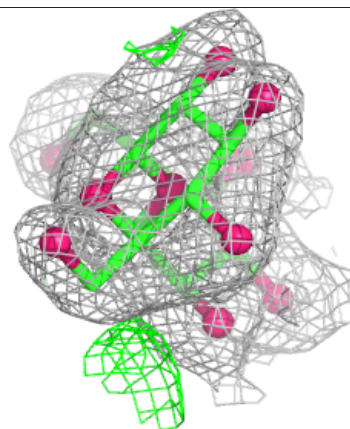
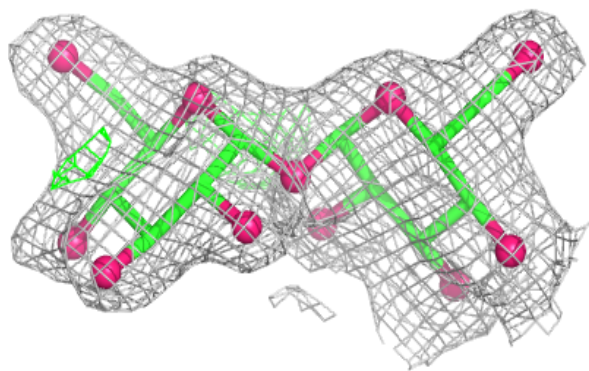
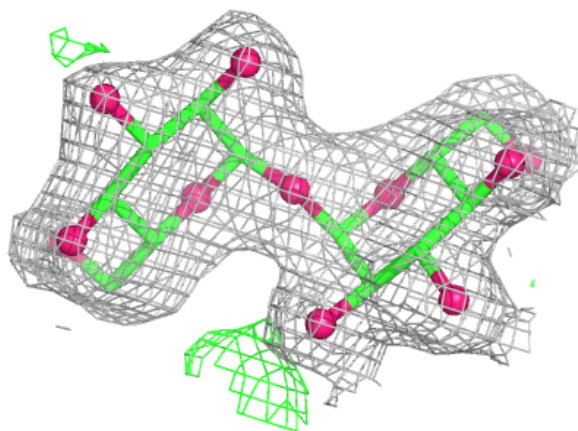
**Electron density around Chain q:**

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



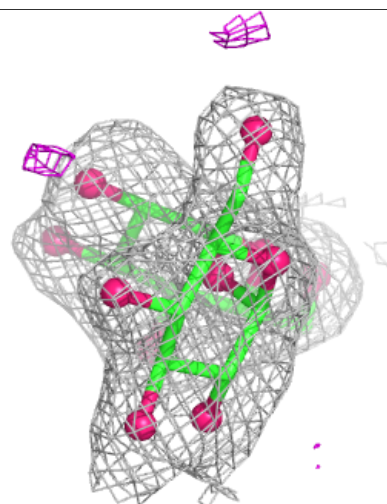
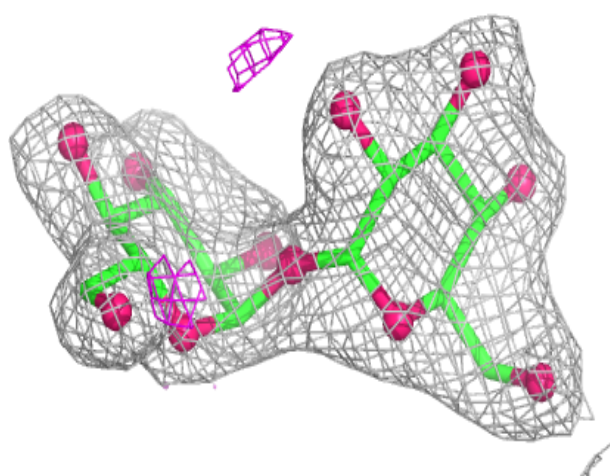
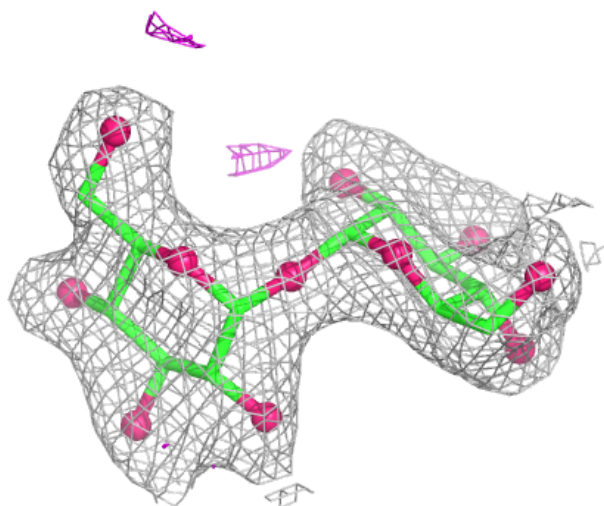
Electron density around Chain s:

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



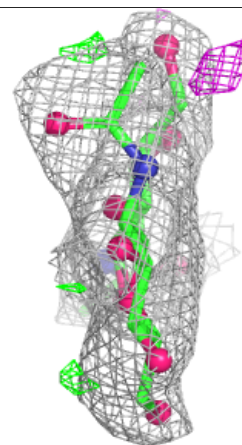
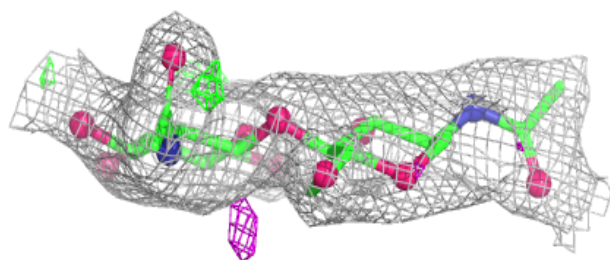
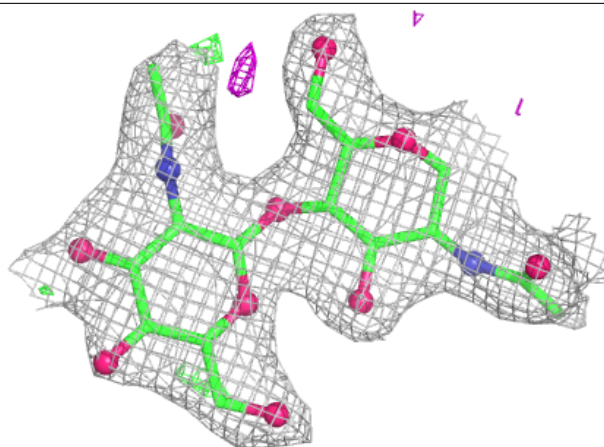
Electron density around Chain u:

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



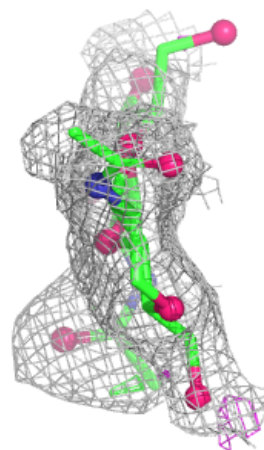
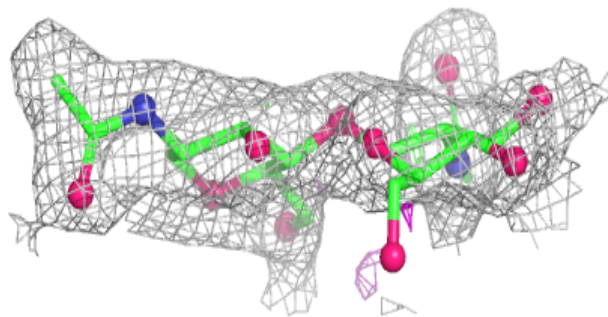
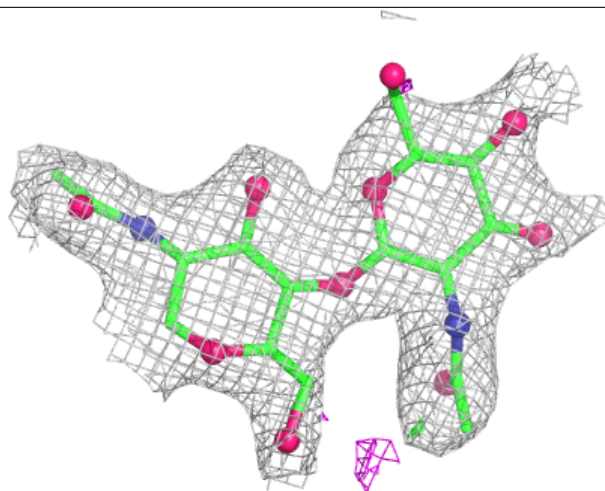
Electron density around Chain R:

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



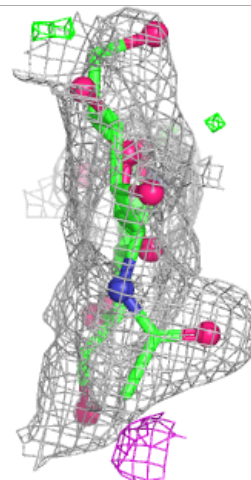
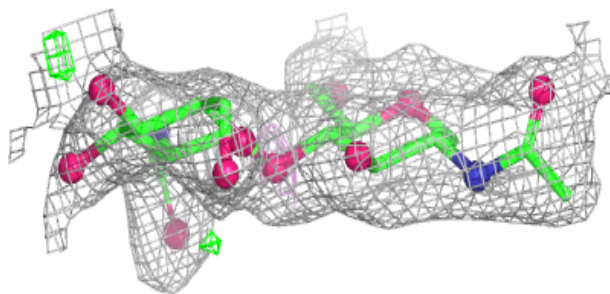
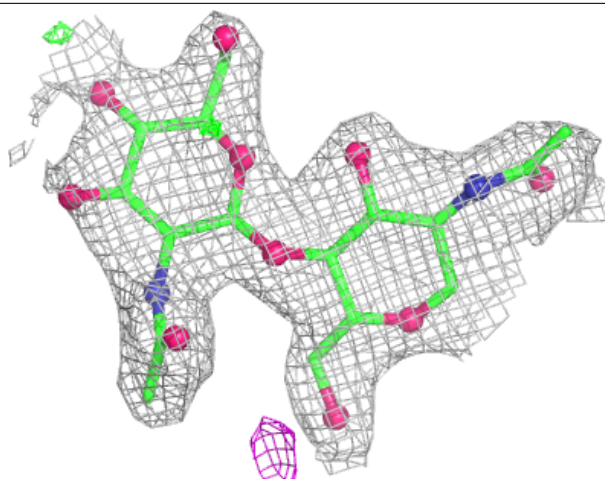
Electron density around Chain V:

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



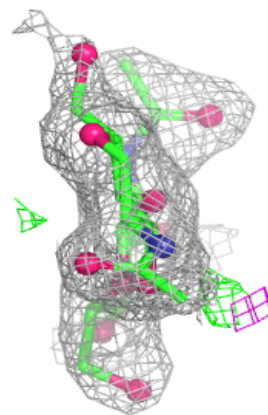
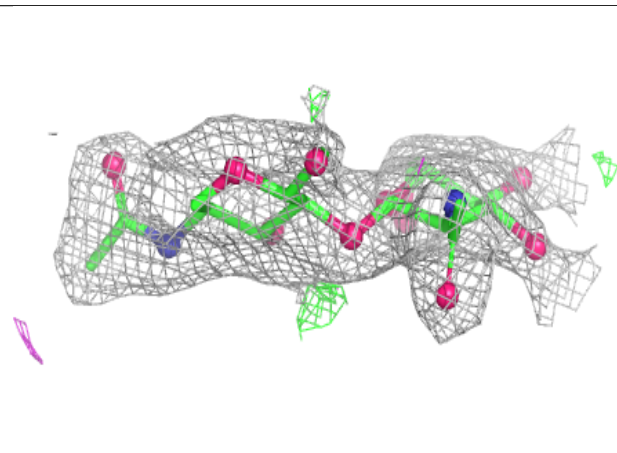
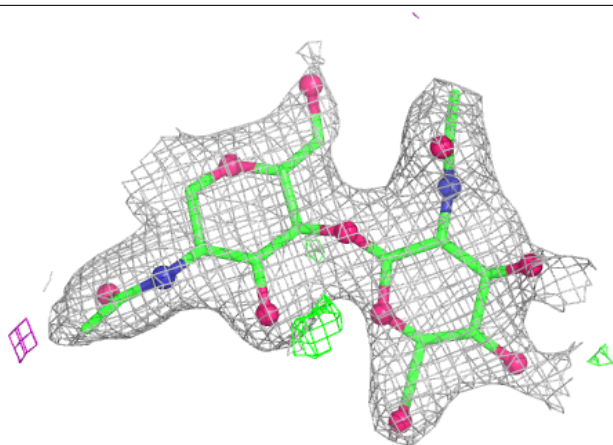
Electron density around Chain Z:

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



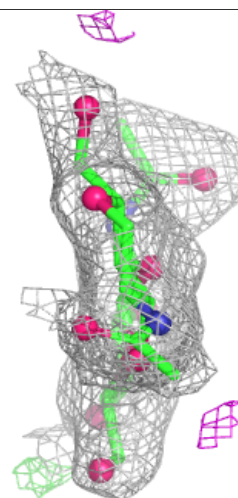
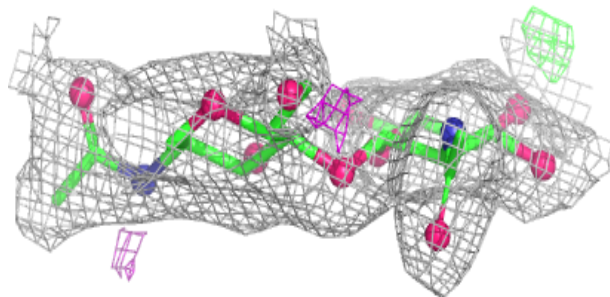
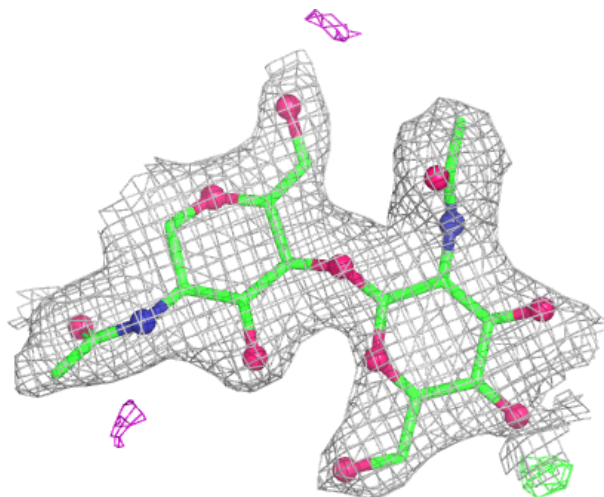
Electron density around Chain d:

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



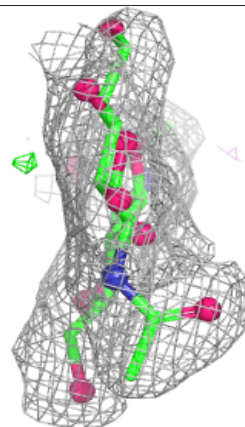
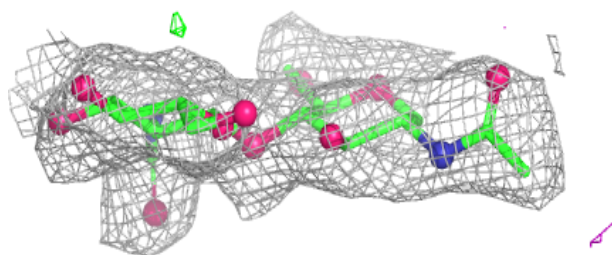
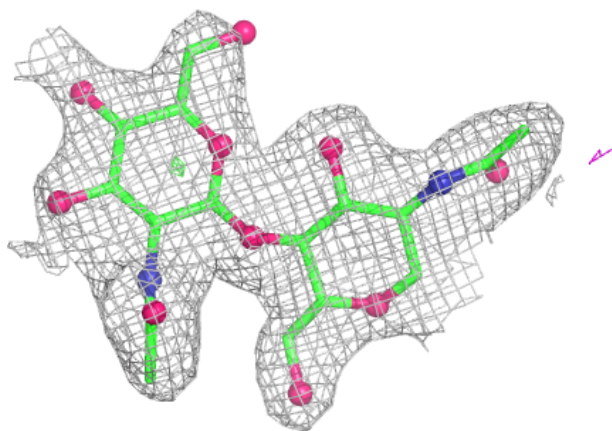
Electron density around Chain h:

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



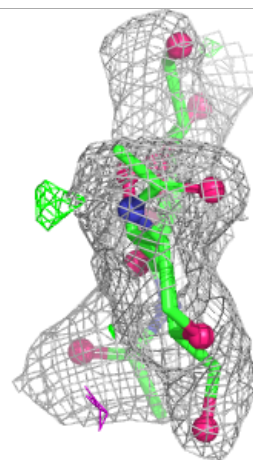
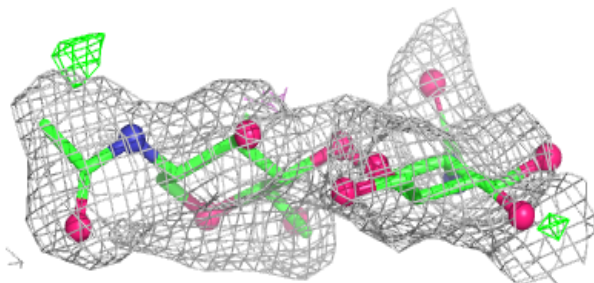
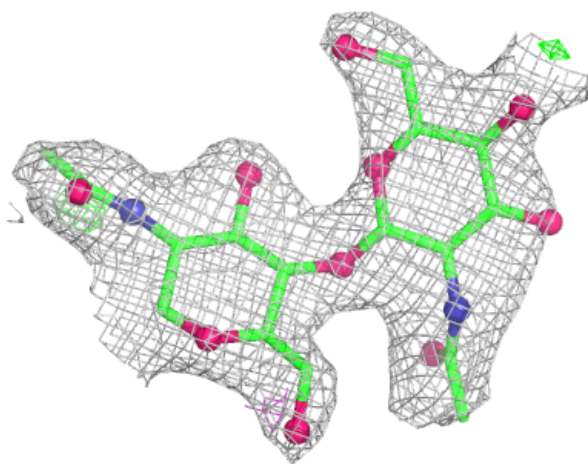
Electron density around Chain 1:

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



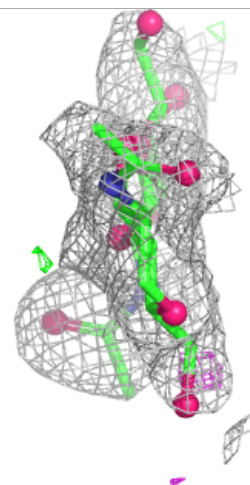
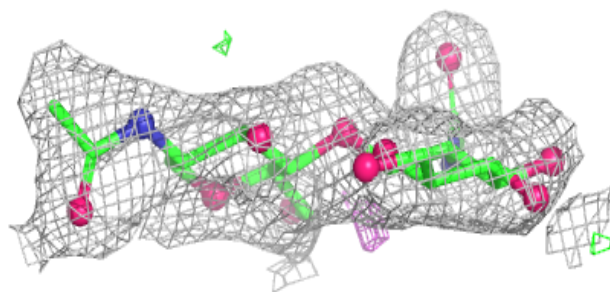
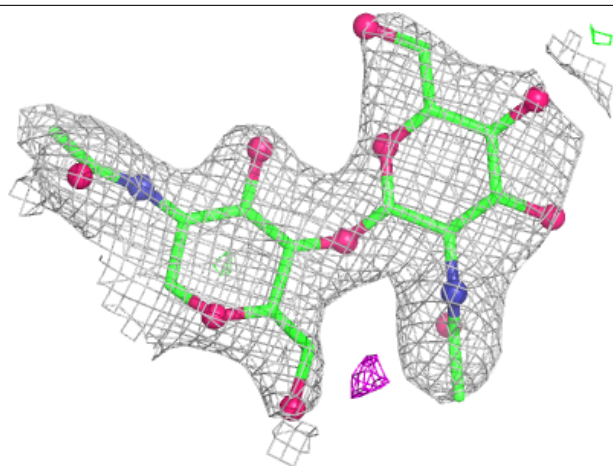
Electron density around Chain p:

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



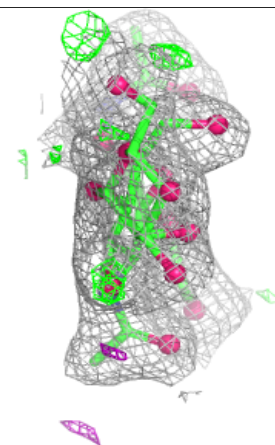
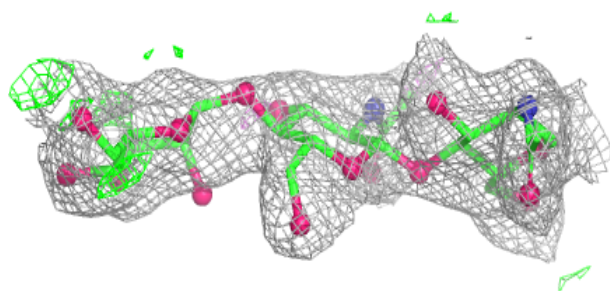
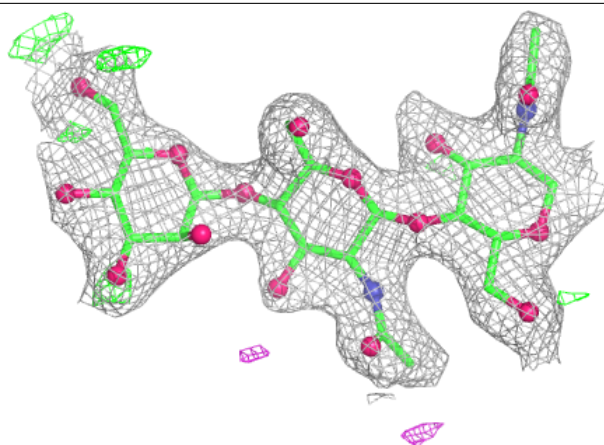
Electron density around Chain t:

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

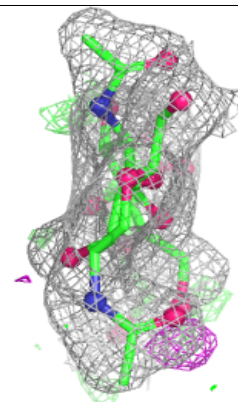
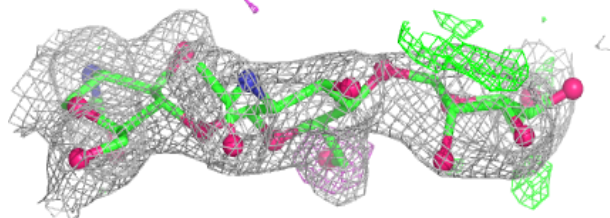
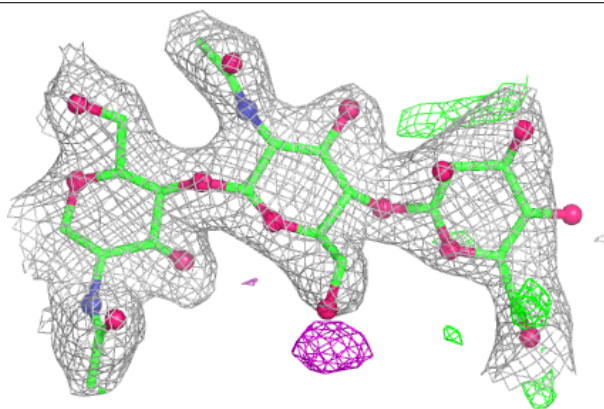


Electron density around Chain T:

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

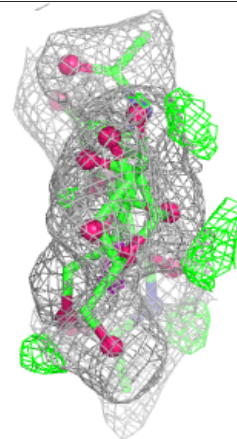
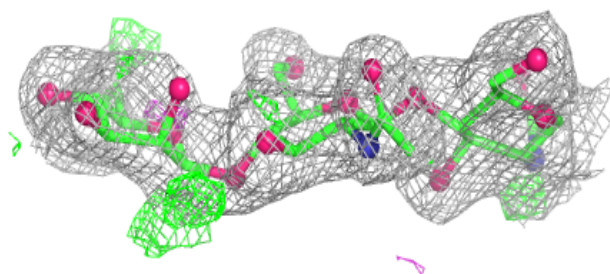
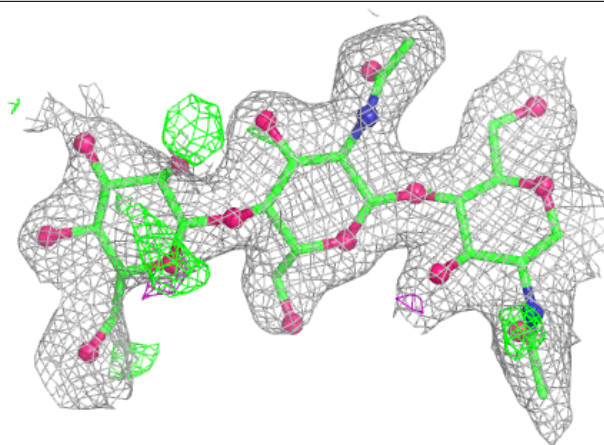
**Electron density around Chain X:**

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

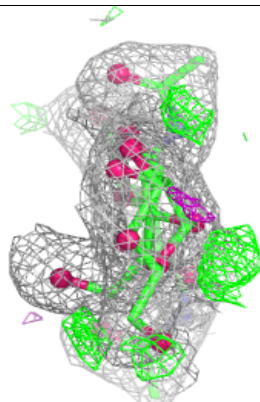
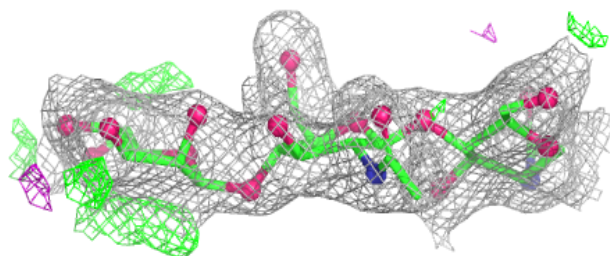
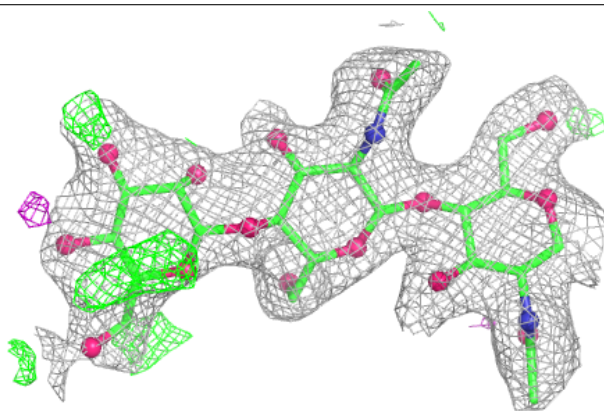


Electron density around Chain b:

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

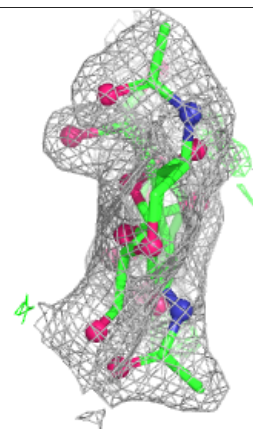
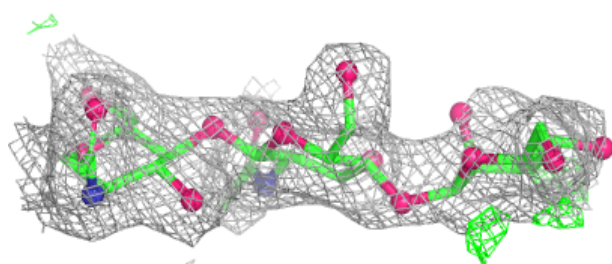
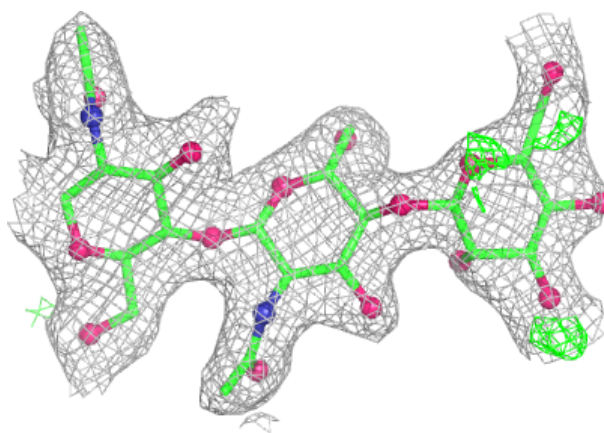
**Electron density around Chain f:**

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

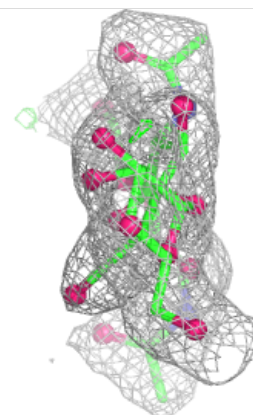
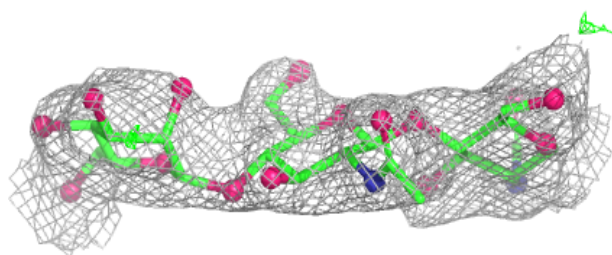
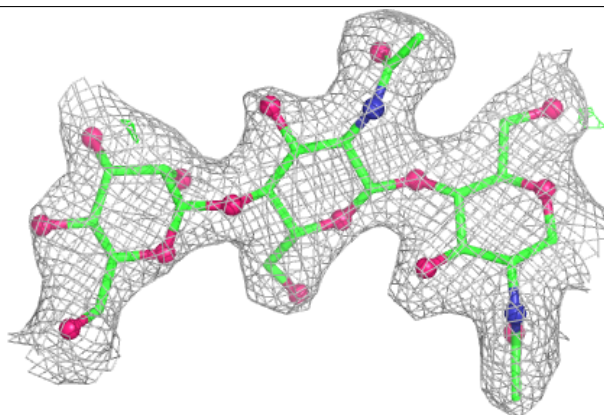


Electron density around Chain j:

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

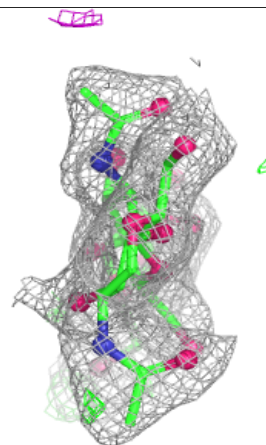
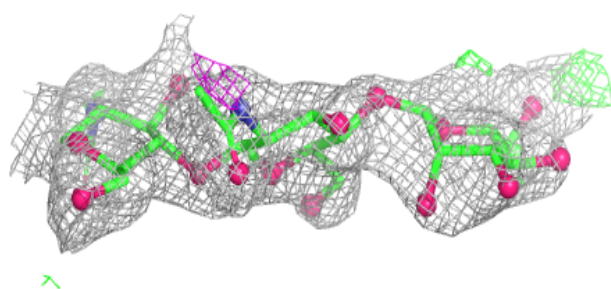
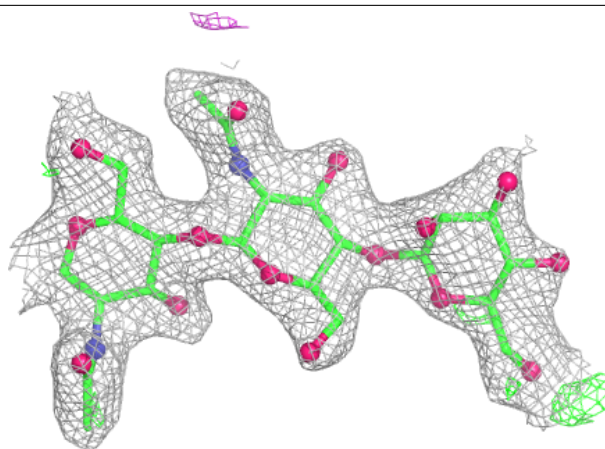
**Electron density around Chain n:**

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

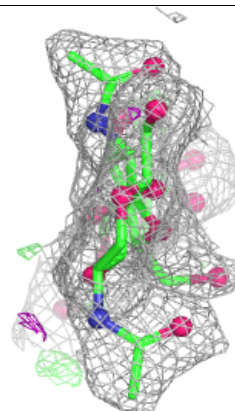
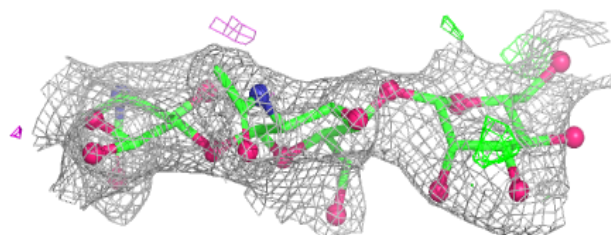
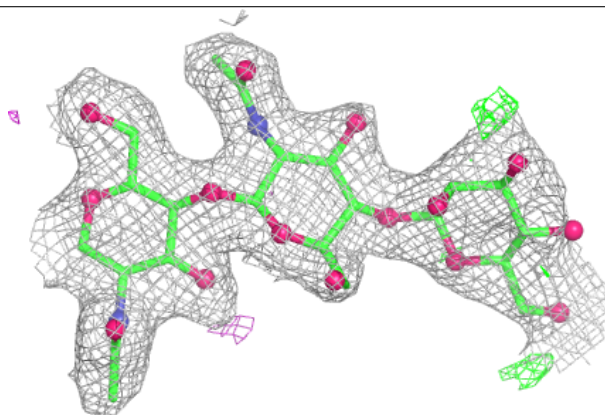


Electron density around Chain r:

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

**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)



6.4 Ligands ⓘ

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
6	NAG	A	501	14/15	0.89	0.11	62,66,74,76	0
6	NAG	G	503	14/15	0.89	0.11	70,78,81,81	0
6	NAG	E	503	14/15	0.90	0.10	69,74,79,79	0
6	NAG	A	503	14/15	0.90	0.10	73,78,82,84	0
6	NAG	I	501	14/15	0.90	0.11	60,67,74,74	0
6	NAG	I	503	14/15	0.90	0.10	69,76,81,82	0
6	NAG	O	503	14/15	0.90	0.10	67,72,77,77	0
6	NAG	M	501	14/15	0.91	0.11	67,72,75,76	0
6	NAG	E	501	14/15	0.91	0.10	71,75,76,77	0
6	NAG	J	1004	14/15	0.92	0.10	62,68,72,72	0
6	NAG	G	501	14/15	0.93	0.09	70,73,75,76	0
6	NAG	C	501	14/15	0.93	0.09	72,78,84,86	0
6	NAG	H	1004	14/15	0.93	0.09	54,60,64,65	0
6	NAG	O	501	14/15	0.93	0.10	71,75,82,84	0
6	NAG	C	503	14/15	0.93	0.08	62,66,69,72	0
8	GLC	C	506	12/12	0.93	0.10	71,74,76,77	0
6	NAG	N	1003	14/15	0.94	0.08	50,53,57,58	0
6	NAG	L	1004	14/15	0.94	0.09	75,78,80,81	0
6	NAG	L	1005	14/15	0.94	0.09	48,58,60,60	0
6	NAG	P	1004	14/15	0.94	0.08	57,61,65,66	0
6	NAG	B	1004	14/15	0.94	0.09	51,58,62,63	0
6	NAG	D	1003	14/15	0.95	0.08	55,59,63,63	0
6	NAG	F	1003	14/15	0.95	0.08	54,58,63,63	0
6	NAG	H	1003	14/15	0.95	0.07	58,63,64,64	0
8	GLC	E	506	12/12	0.95	0.08	54,57,57,58	0
8	GLC	I	506	12/12	0.95	0.08	63,69,70,70	0
8	GLC	L	1002	12/12	0.95	0.07	57,59,61,61	0
6	NAG	C	505	14/15	0.96	0.07	45,55,58,59	0
6	NAG	O	504	14/15	0.96	0.07	46,49,51,51	0
6	NAG	C	504	14/15	0.96	0.07	48,50,53,54	0
8	GLC	B	1002	12/12	0.96	0.07	52,56,57,57	0
6	NAG	M	503	14/15	0.96	0.06	49,51,53,53	0
6	NAG	M	504	14/15	0.96	0.06	45,47,50,51	0
8	GLC	G	506	12/12	0.96	0.07	53,58,59,60	0
6	NAG	K	503	14/15	0.96	0.06	44,47,49,50	0
6	NAG	E	504	14/15	0.96	0.07	50,54,57,57	0
8	GLC	M	506	12/12	0.96	0.07	50,54,55,55	0

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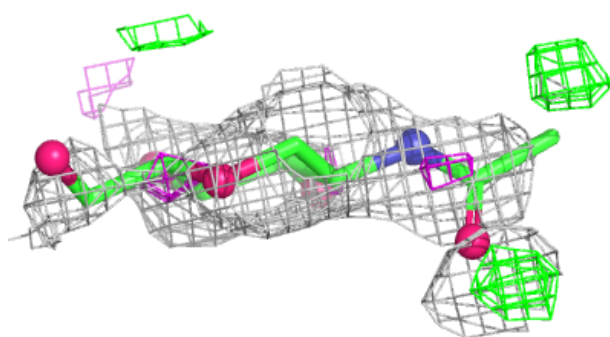
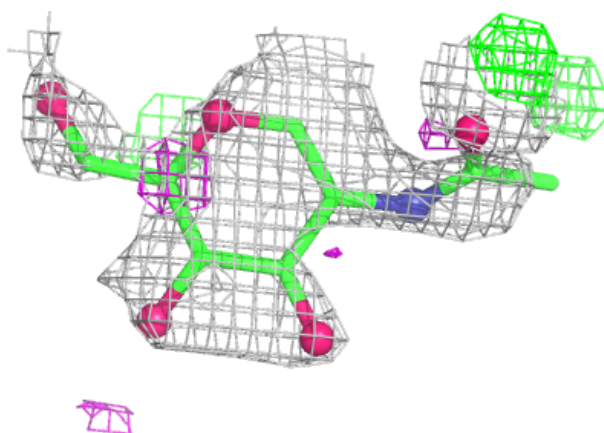
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GLC	P	1002	12/12	0.96	0.07	60,62,63,63	0
6	NAG	D	1002	14/15	0.97	0.06	47,50,51,52	0
6	NAG	O	505	14/15	0.97	0.06	42,48,52,53	0
6	NAG	P	1003	14/15	0.97	0.06	47,50,53,53	0
6	NAG	A	505	14/15	0.97	0.06	36,40,42,43	0
6	NAG	G	504	14/15	0.97	0.06	47,50,53,54	0
6	NAG	I	504	14/15	0.97	0.06	42,43,45,46	0
6	NAG	I	505	14/15	0.97	0.06	38,41,44,46	0
6	NAG	M	505	14/15	0.97	0.06	40,43,45,47	0
6	NAG	J	1003	14/15	0.97	0.07	53,57,60,63	0
6	NAG	G	505	14/15	0.97	0.07	42,44,49,49	0
6	NAG	O	502	14/15	0.97	0.06	40,44,47,48	0
6	NAG	A	504	14/15	0.97	0.06	42,44,46,46	0
6	NAG	H	1002	14/15	0.98	0.04	42,44,45,45	0
6	NAG	K	501	14/15	0.98	0.05	42,45,47,47	0
6	NAG	K	502	14/15	0.98	0.05	43,45,46,46	0
6	NAG	F	1002	14/15	0.98	0.05	40,43,44,45	0
6	NAG	L	1003	14/15	0.98	0.06	46,49,52,52	0
6	NAG	C	502	14/15	0.98	0.05	40,42,43,44	0
6	NAG	E	502	14/15	0.98	0.05	36,38,41,41	0
6	NAG	I	502	14/15	0.98	0.05	38,39,42,44	0
6	NAG	G	502	14/15	0.98	0.05	38,42,44,45	0
6	NAG	A	502	14/15	0.98	0.05	38,40,41,43	0
6	NAG	B	1003	14/15	0.98	0.04	41,43,44,44	0
6	NAG	N	1002	14/15	0.98	0.05	42,43,44,44	0
6	NAG	J	1002	14/15	0.98	0.04	43,44,45,46	0
6	NAG	E	505	14/15	0.98	0.05	43,50,52,53	0
6	NAG	M	502	14/15	0.99	0.04	34,39,40,42	0
7	NA	B	1001	1/1	1.00	0.04	12,12,12,12	0
7	NA	D	1001	1/1	1.00	0.02	16,16,16,16	0
7	NA	F	1001	1/1	1.00	0.04	17,17,17,17	0
7	NA	H	1001	1/1	1.00	0.03	16,16,16,16	0
7	NA	J	1001	1/1	1.00	0.02	14,14,14,14	0
7	NA	L	1001	1/1	1.00	0.05	18,18,18,18	0
7	NA	N	1001	1/1	1.00	0.02	12,12,12,12	0
7	NA	P	1001	1/1	1.00	0.02	20,20,20,20	0

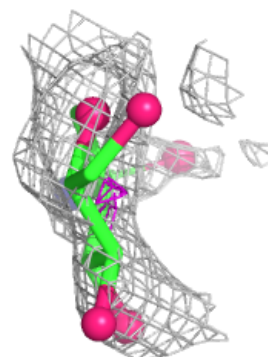
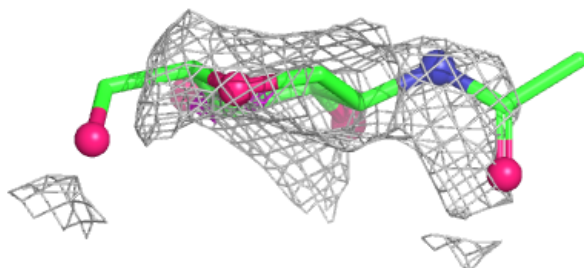
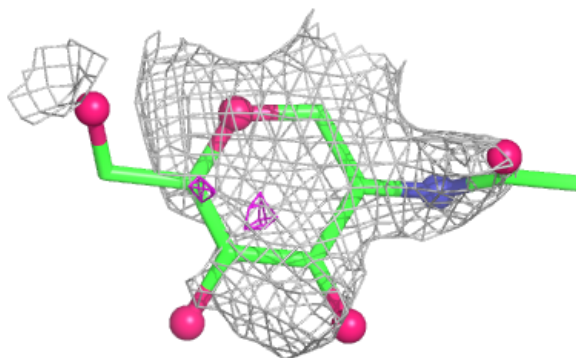
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

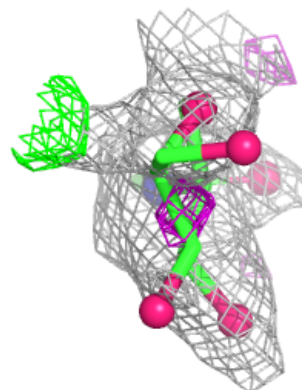
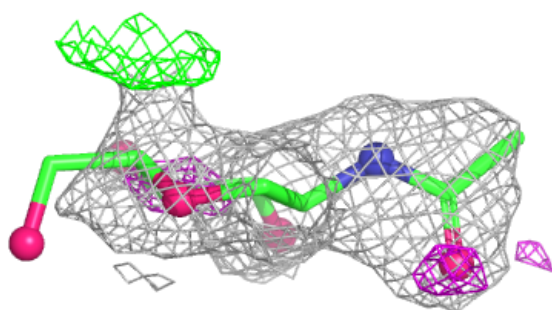
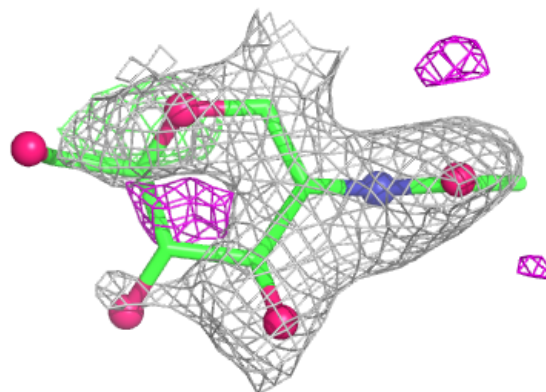
**Electron density around NAG G 503:**

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

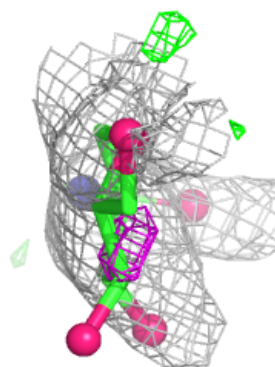
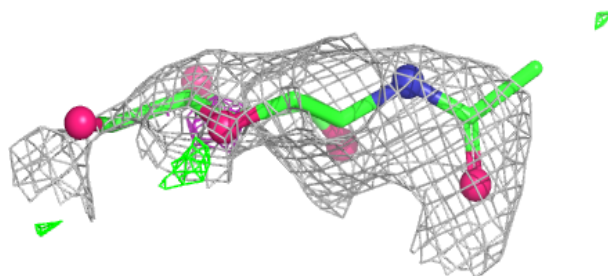
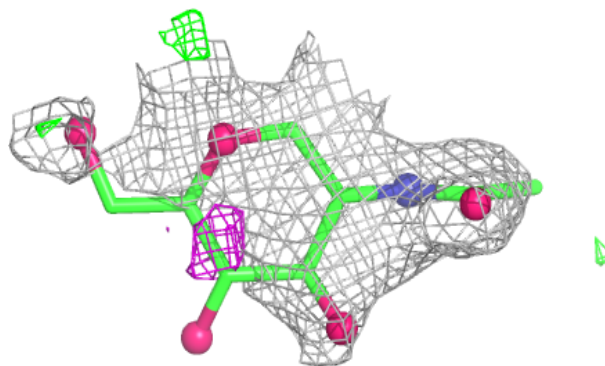


Electron density around NAG E 503:

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

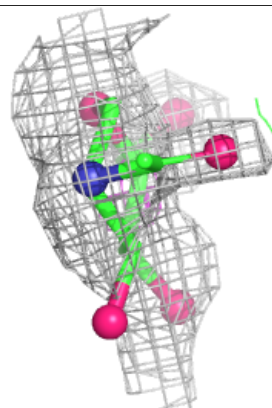
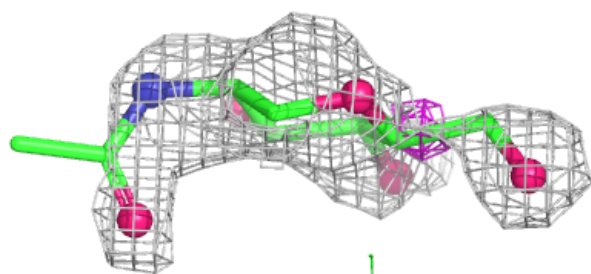
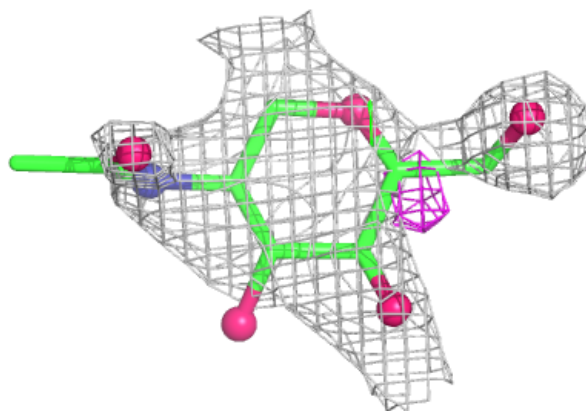
**Electron density around NAG A 503:**

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

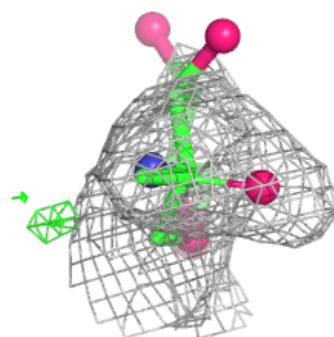
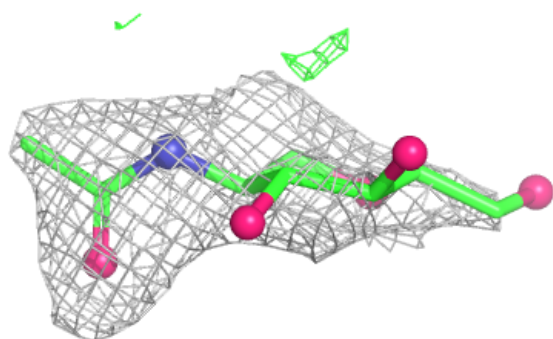
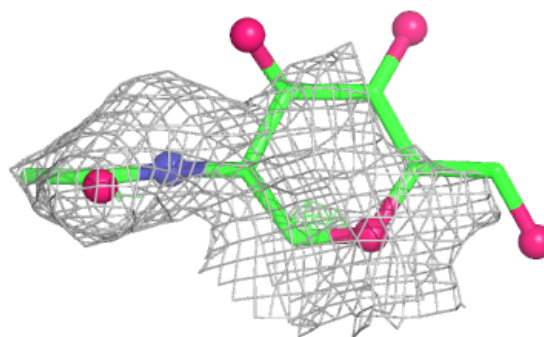


Electron density around NAG I 501:

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

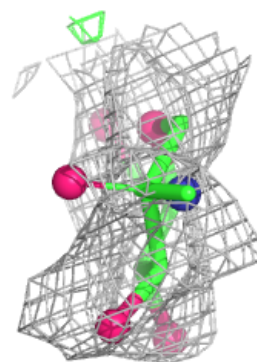
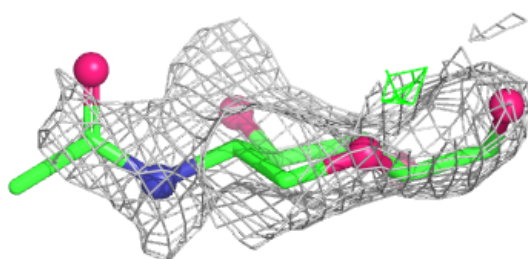
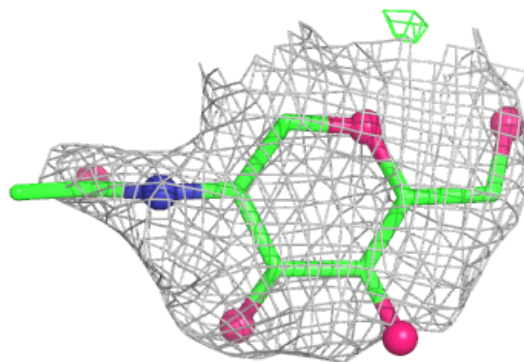
**Electron density around NAG I 503:**

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

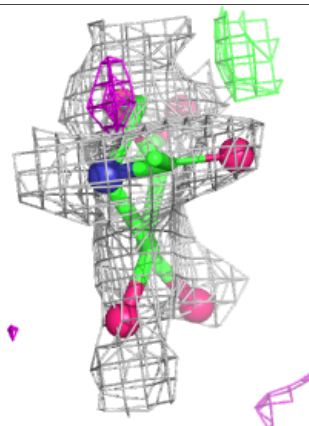
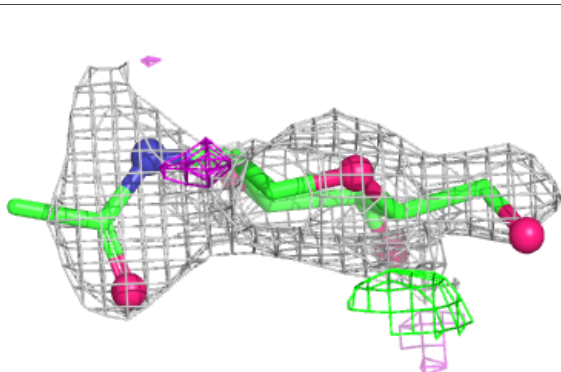


Electron density around NAG O 503:

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

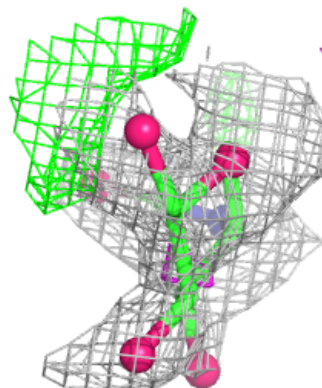
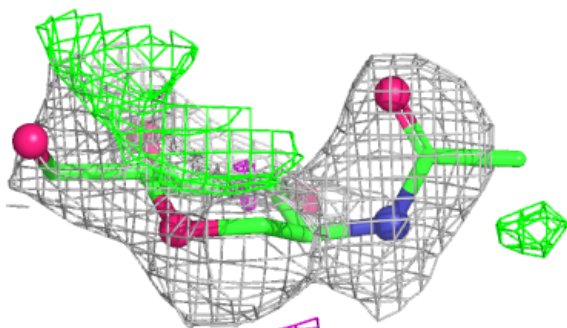
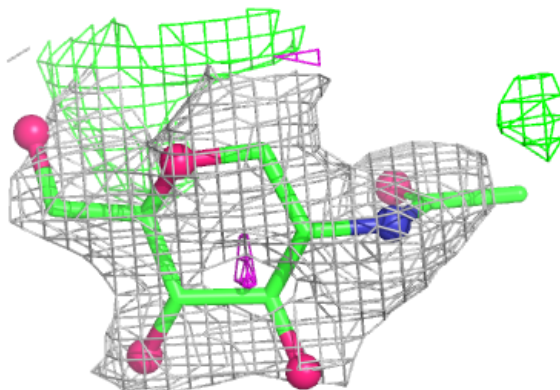
**Electron density around NAG M 501:**

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

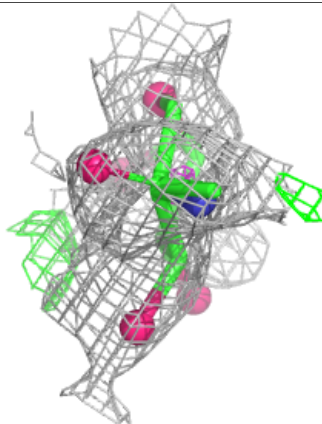
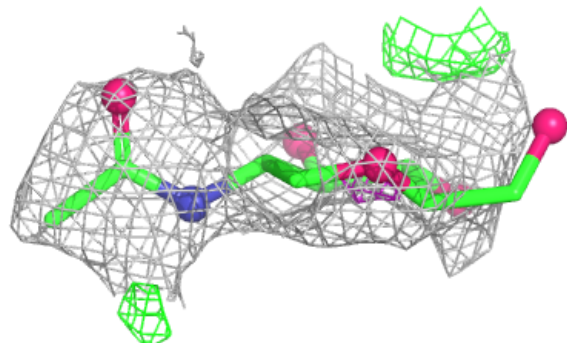
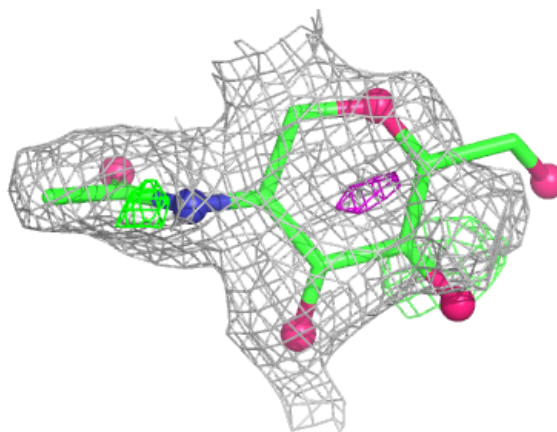


Electron density around NAG E 501:

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

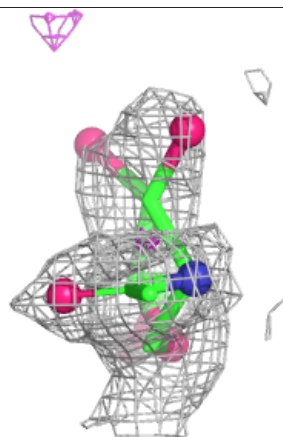
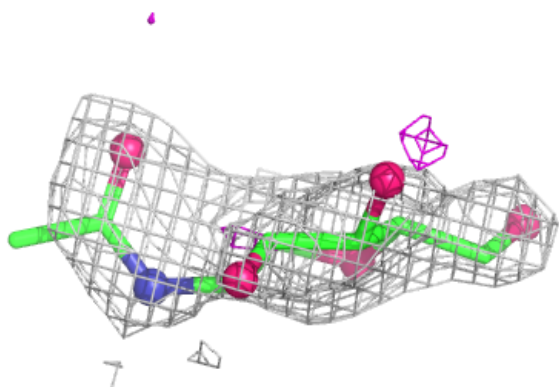
**Electron density around NAG J 1004:**

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



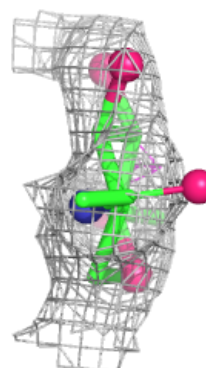
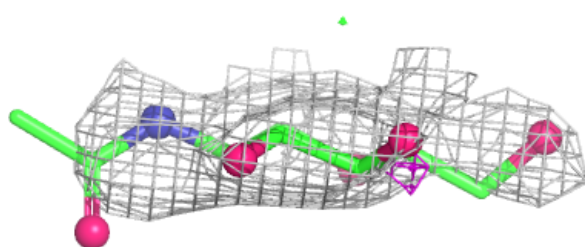
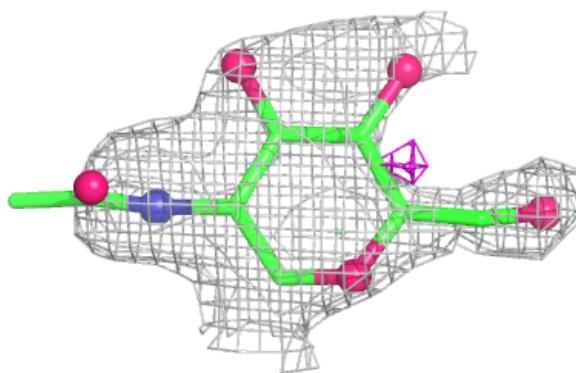
Electron density around NAG G 501:

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

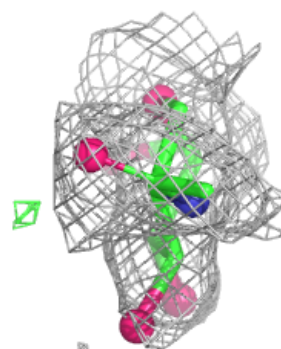
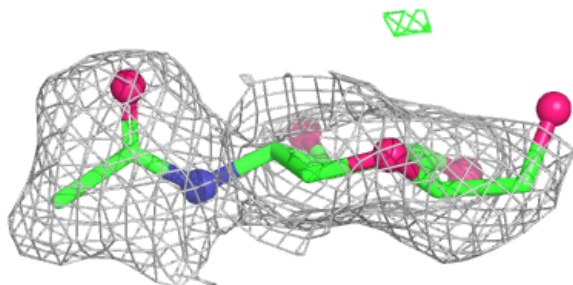
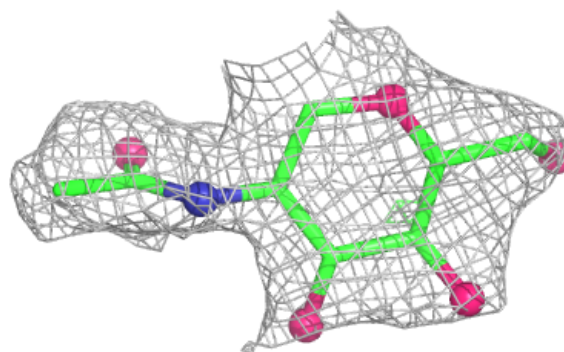


Electron density around NAG C 501:

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

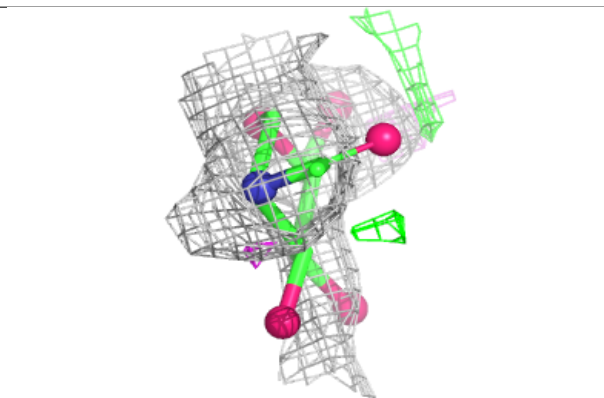
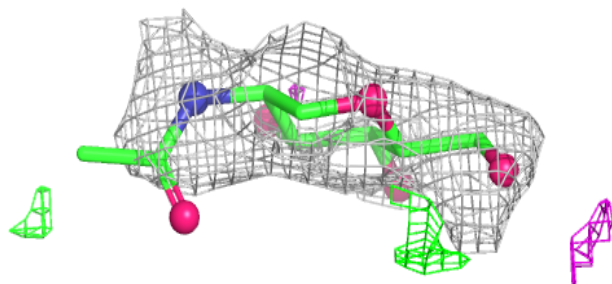
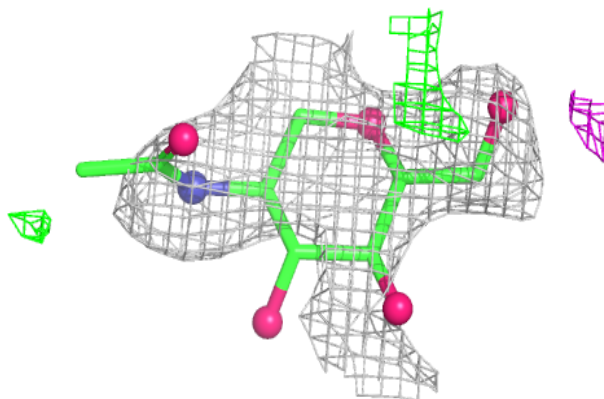
**Electron density around NAG H 1004:**

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

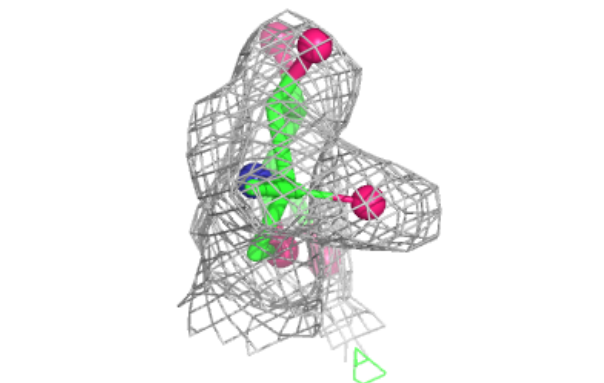
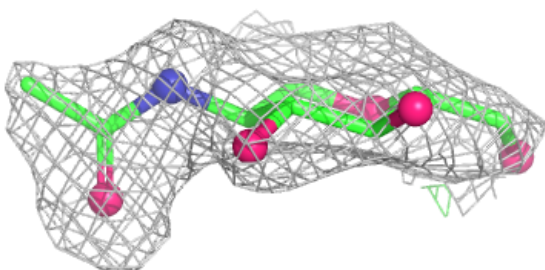
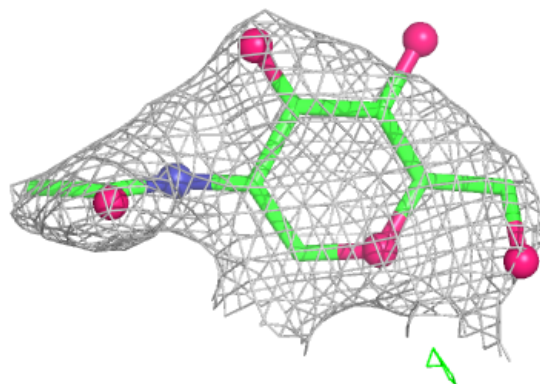


Electron density around NAG O 501:

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

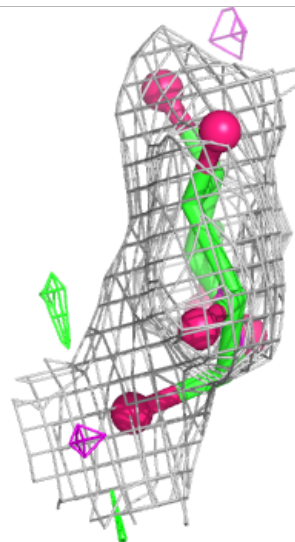
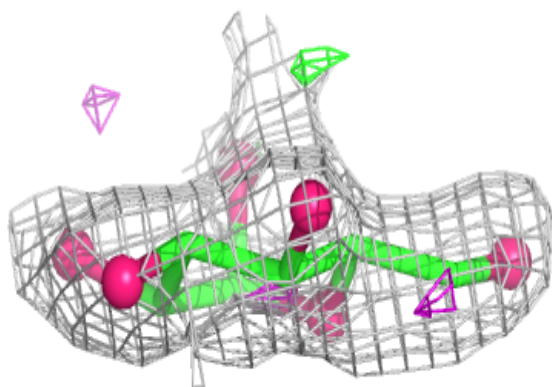
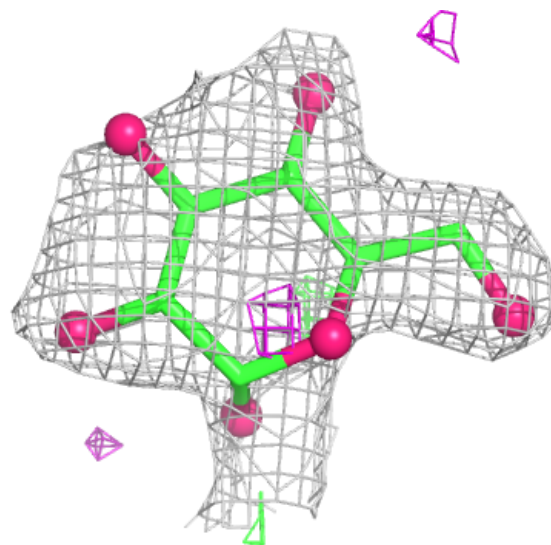
**Electron density around NAG C 503:**

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



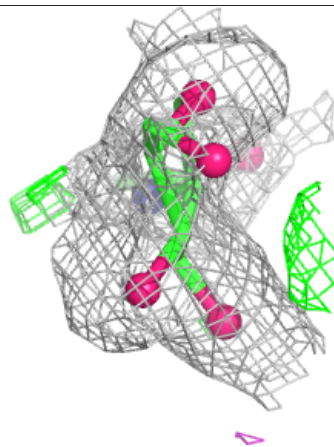
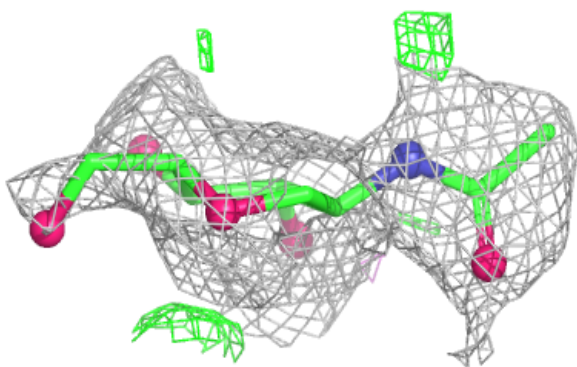
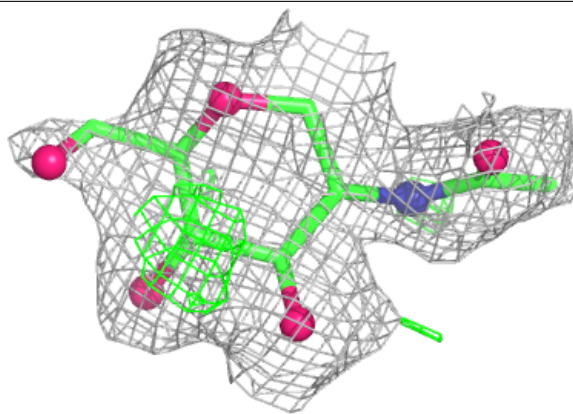
Electron density around GLC C 506:

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



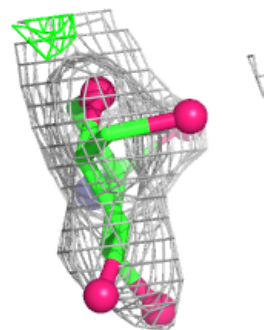
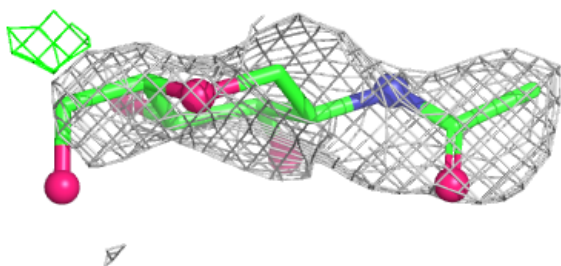
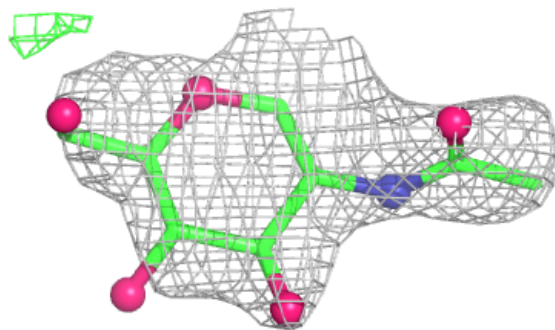
Electron density around NAG N 1003:

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



Electron density around NAG L 1004:

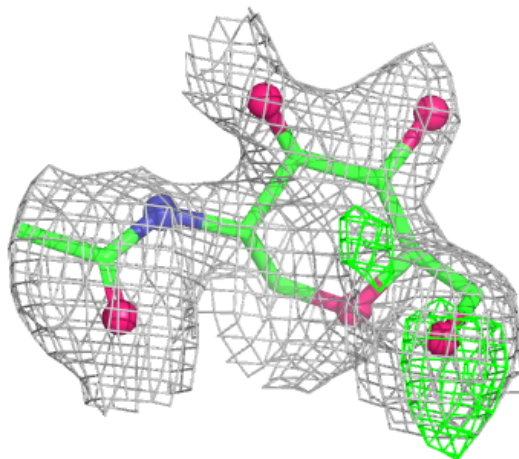
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



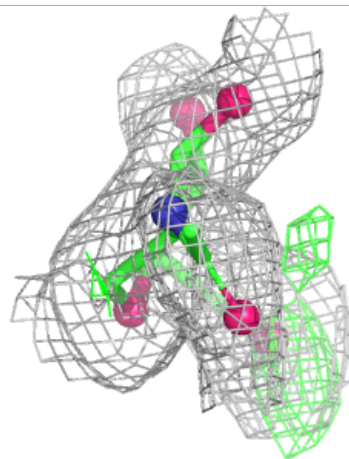
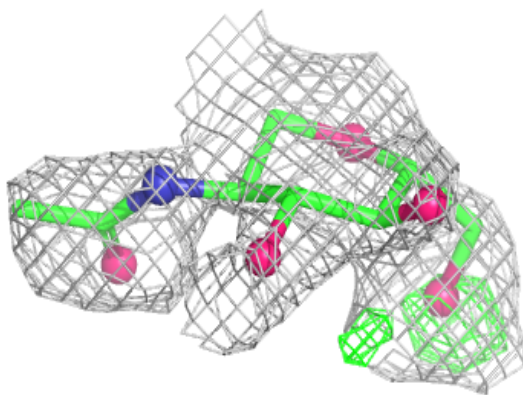
Electron density around NAG L 1005:

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

A

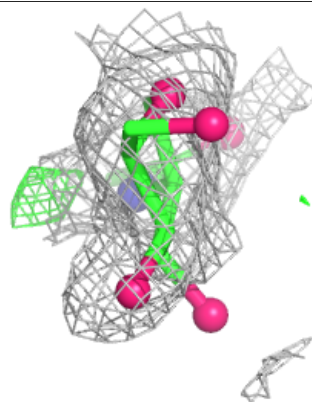
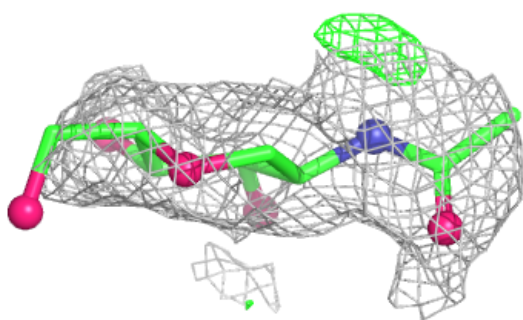
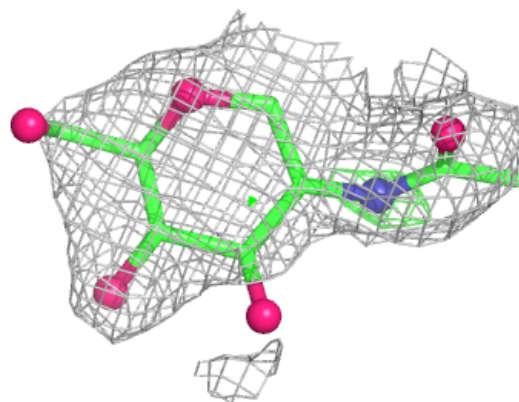


A

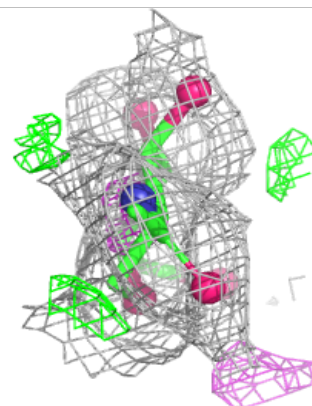
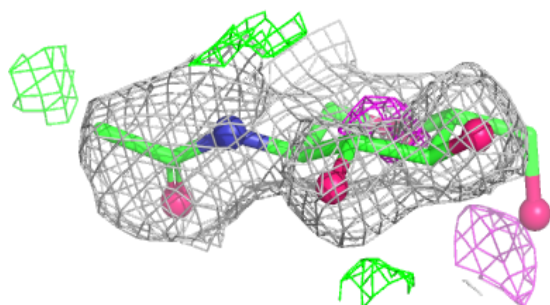
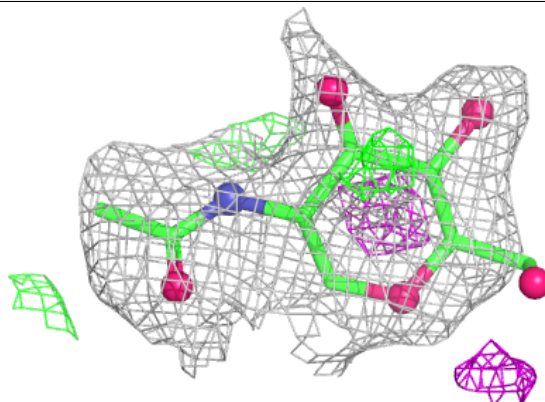


Electron density around NAG P 1004:

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

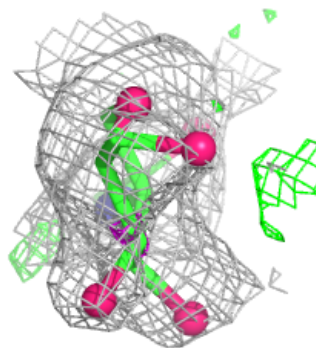
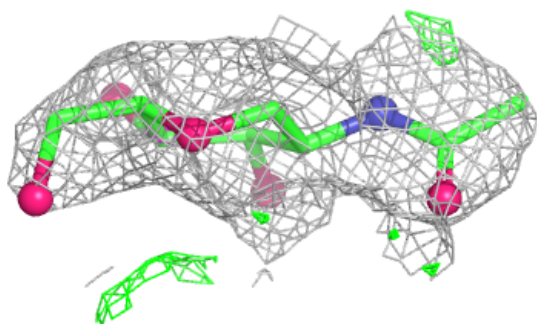
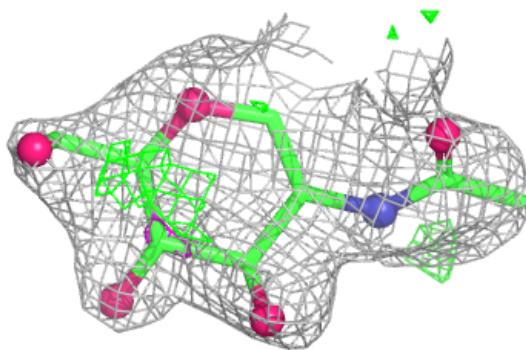
**Electron density around NAG B 1004:**

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

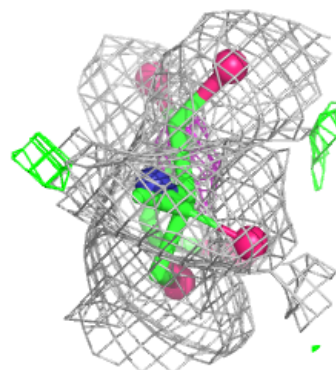
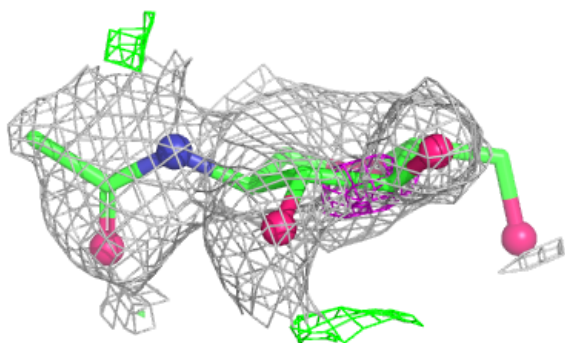
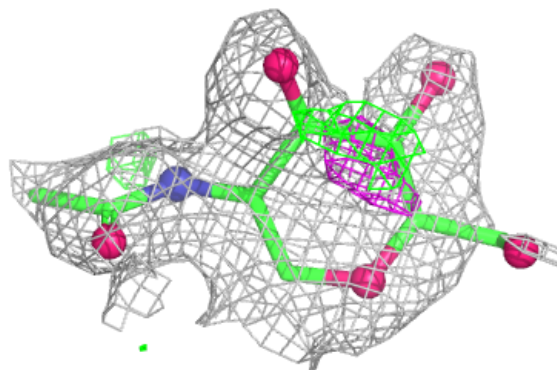


Electron density around NAG D 1003:

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

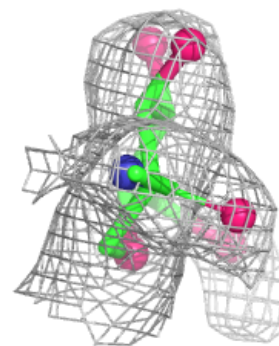
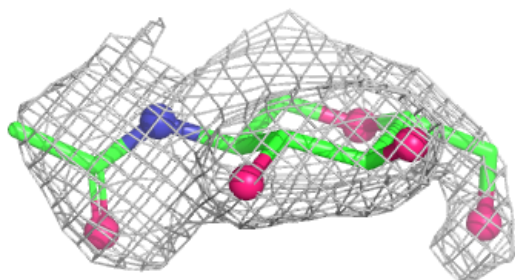
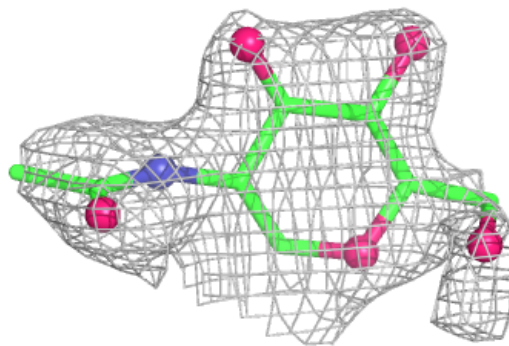
**Electron density around NAG F 1003:**

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



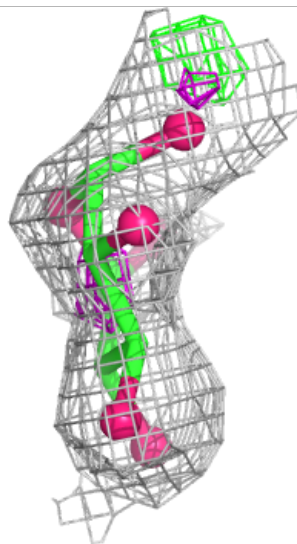
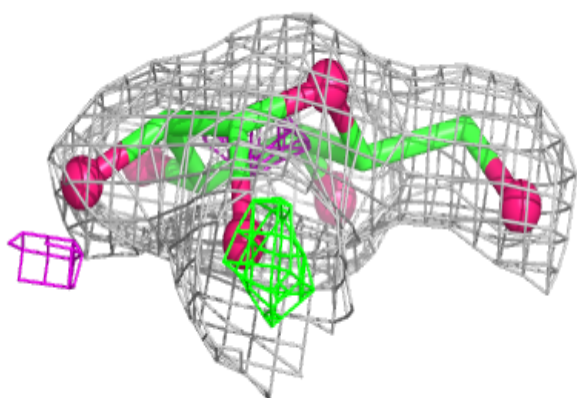
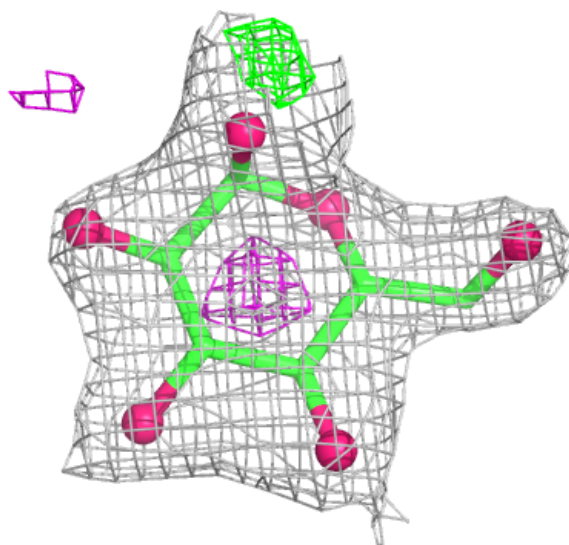
Electron density around NAG H 1003:

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



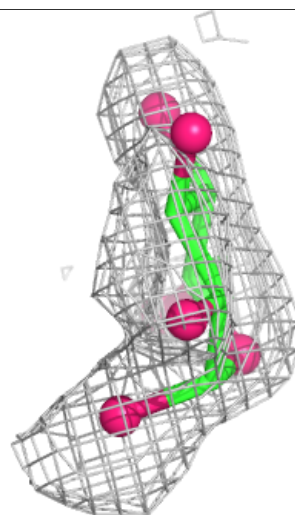
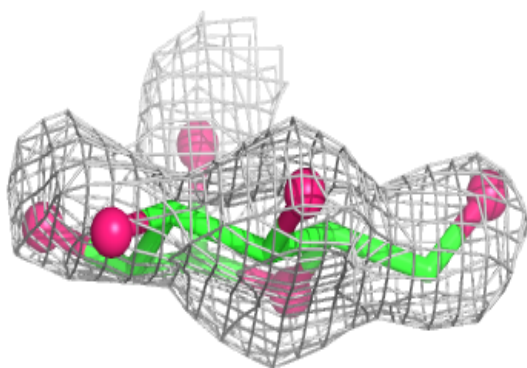
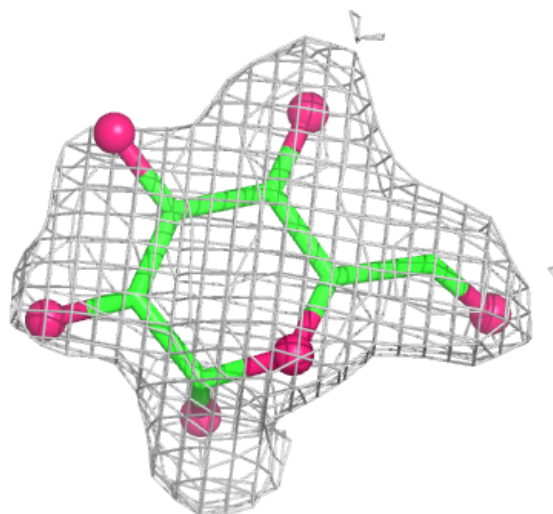
Electron density around GLC E 506:

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



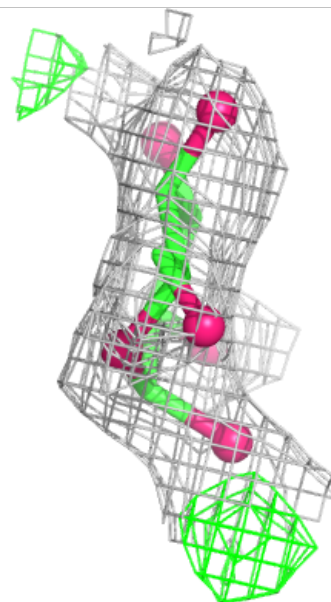
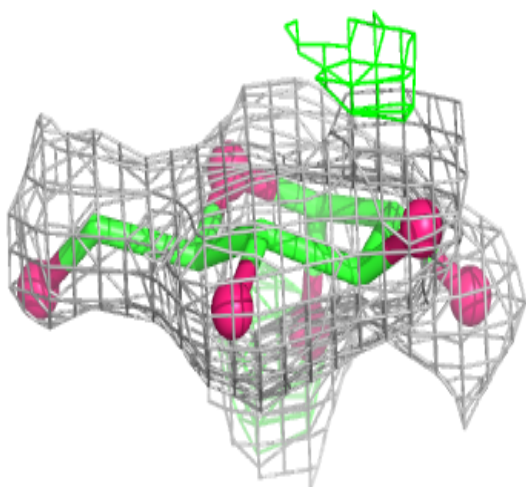
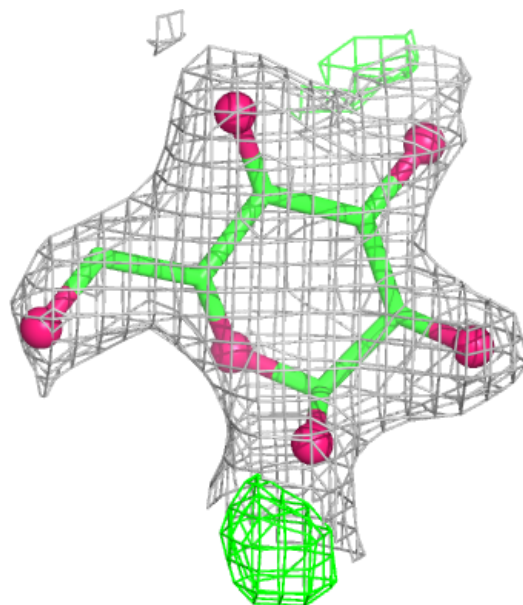
Electron density around GLC I 506:

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



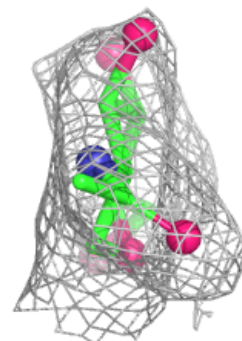
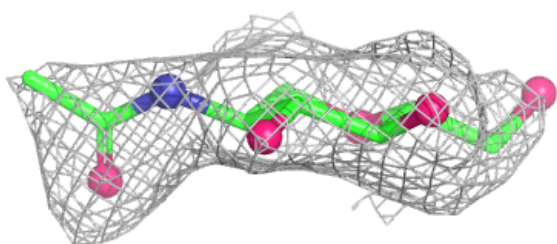
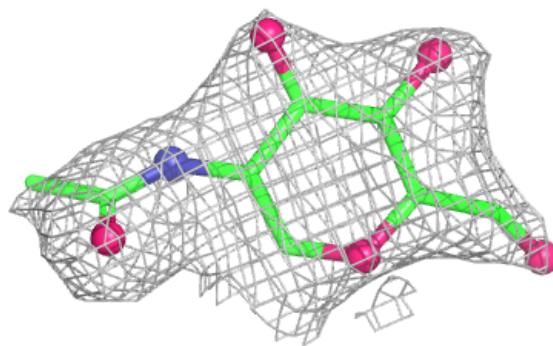
Electron density around GLC L 1002:

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

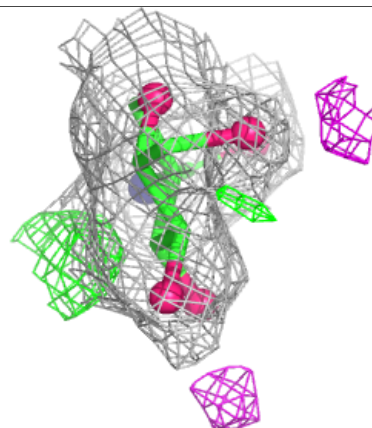
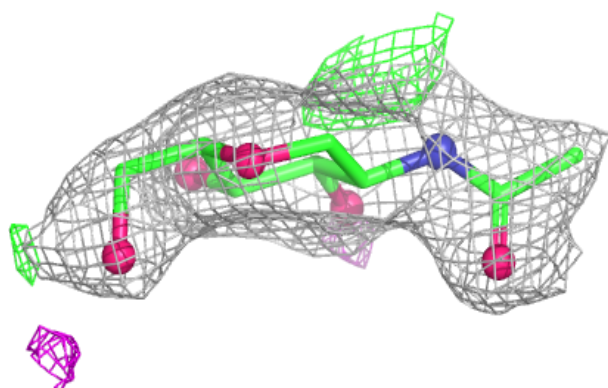
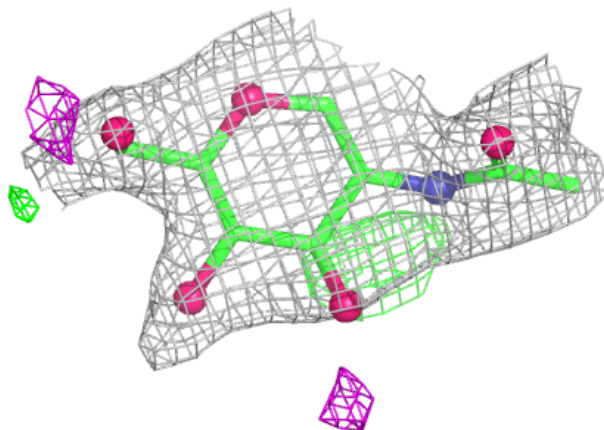


Electron density around NAG C 505:

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

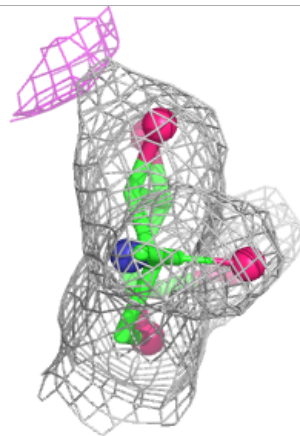
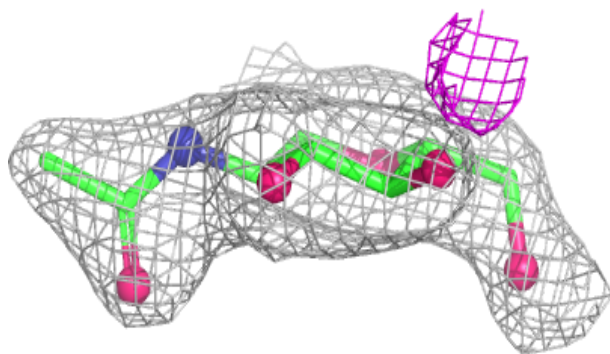
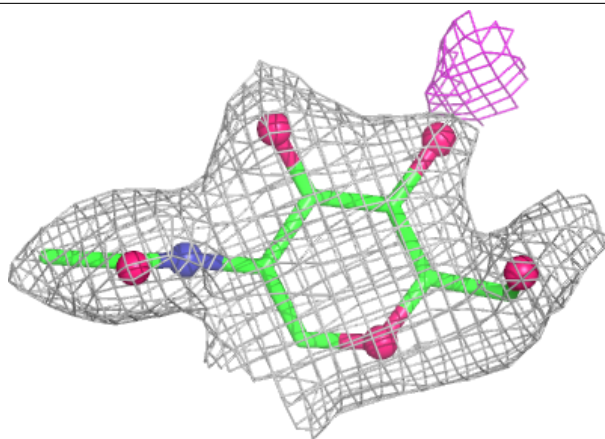
**Electron density around NAG O 504:**

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



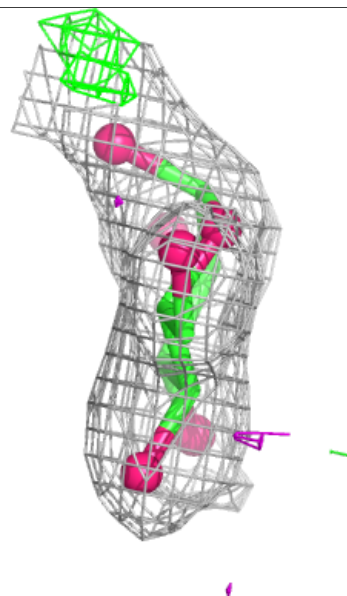
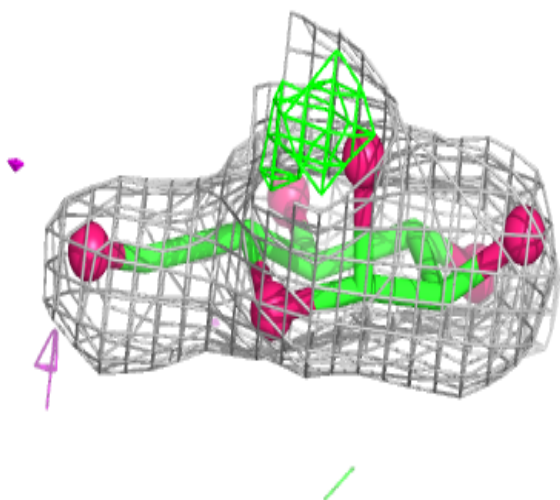
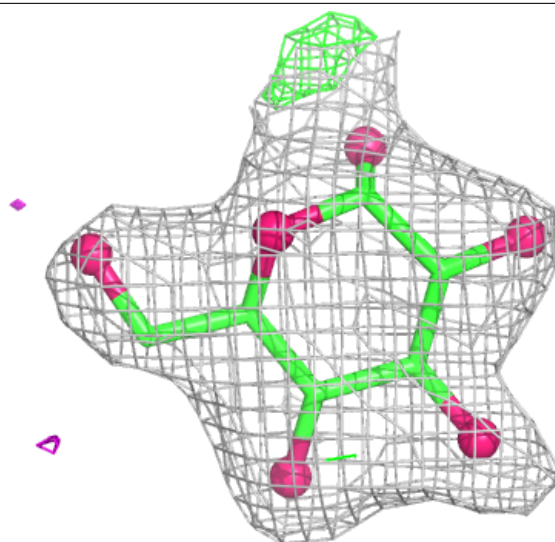
Electron density around NAG C 504:

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



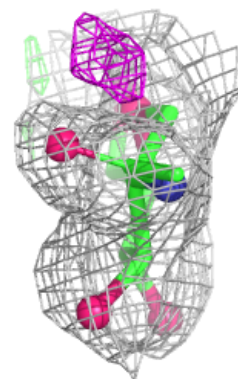
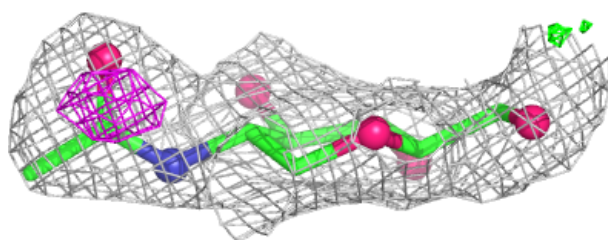
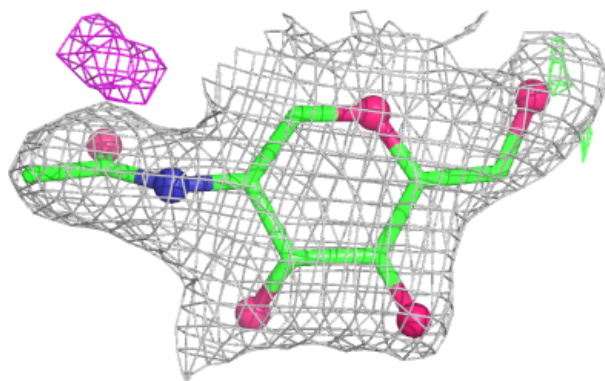
Electron density around GLC B 1002:

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

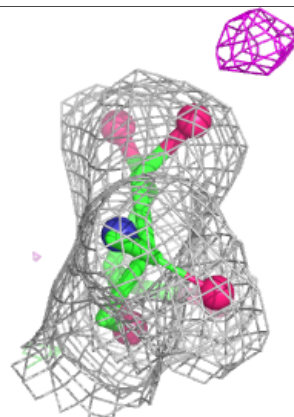
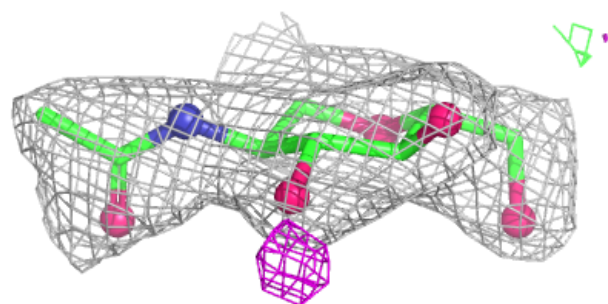
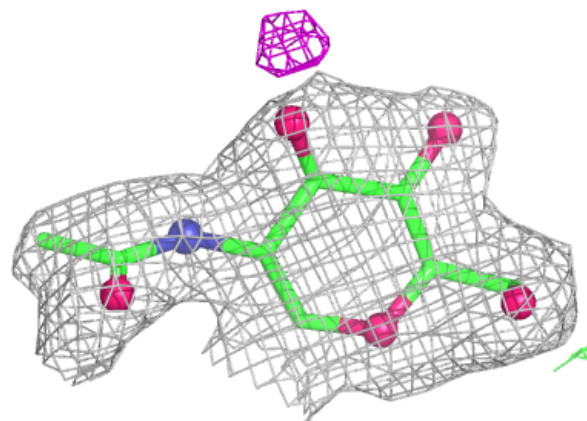


Electron density around NAG M 503:

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

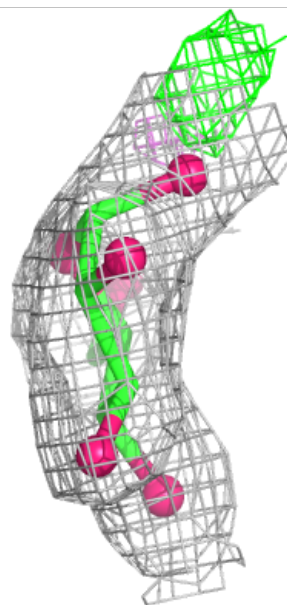
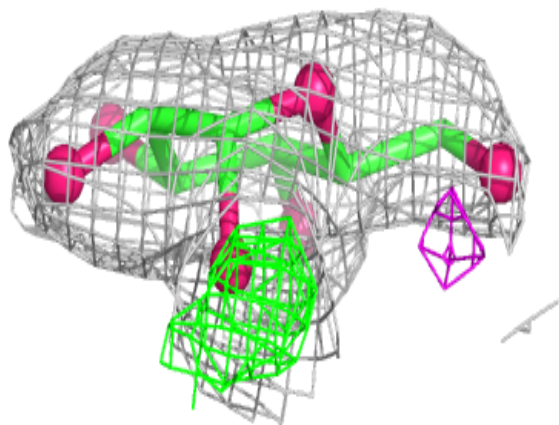
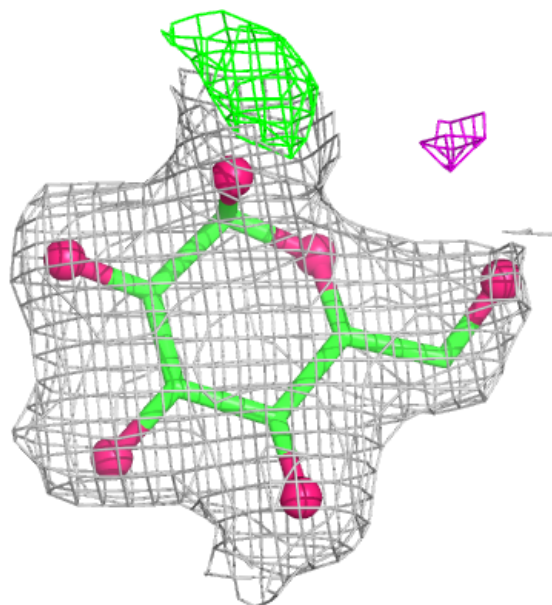
**Electron density around NAG M 504:**

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



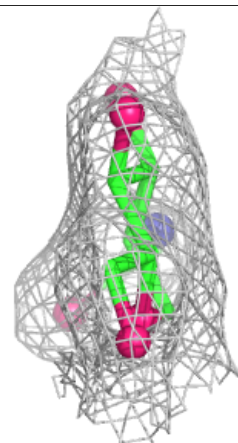
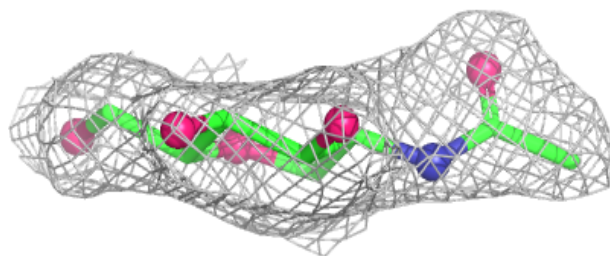
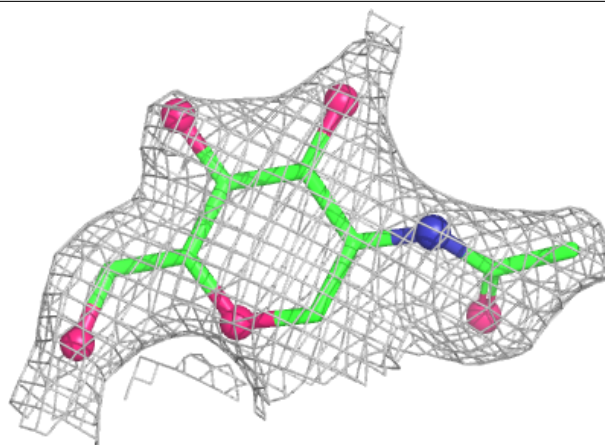
Electron density around GLC G 506:

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

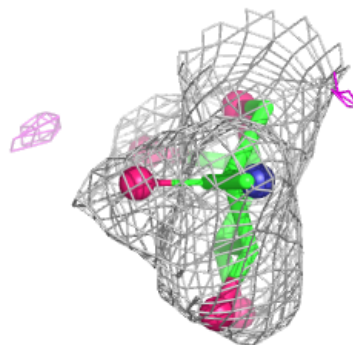
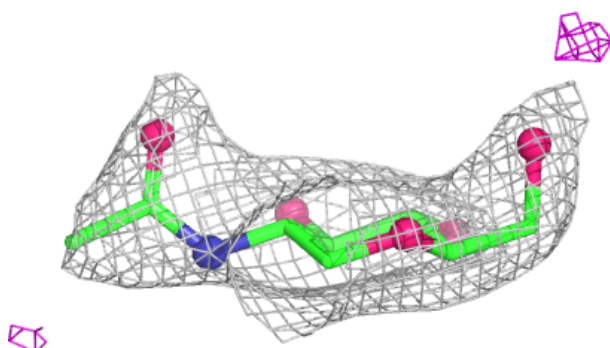
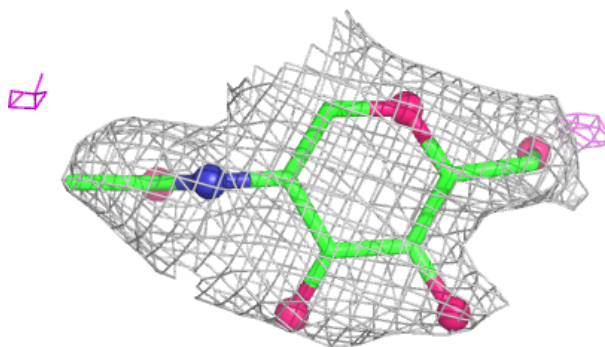


Electron density around NAG K 503:

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

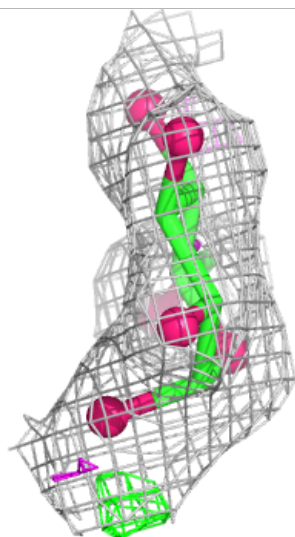
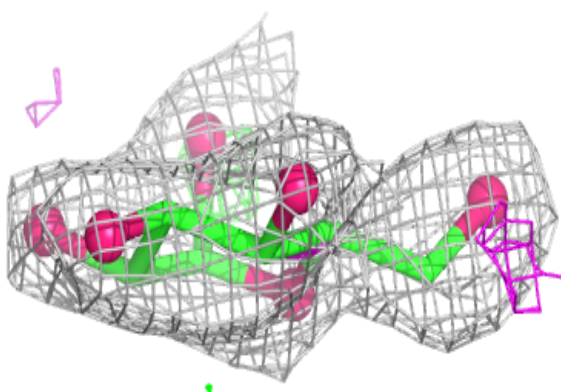
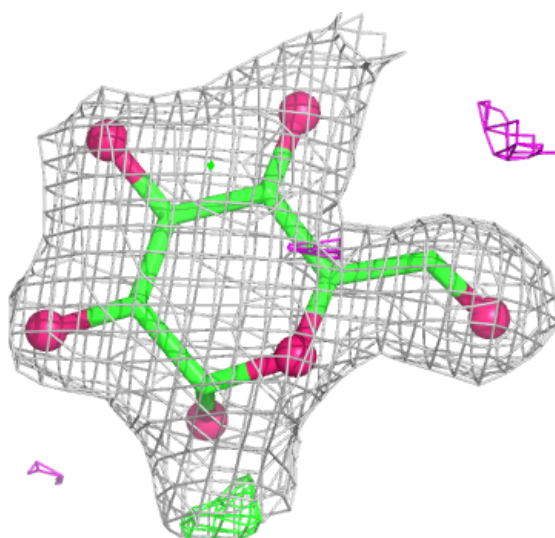
**Electron density around NAG E 504:**

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



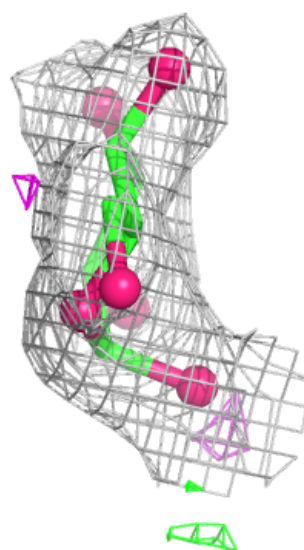
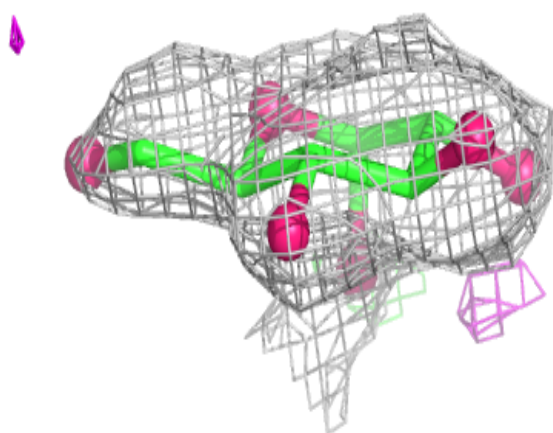
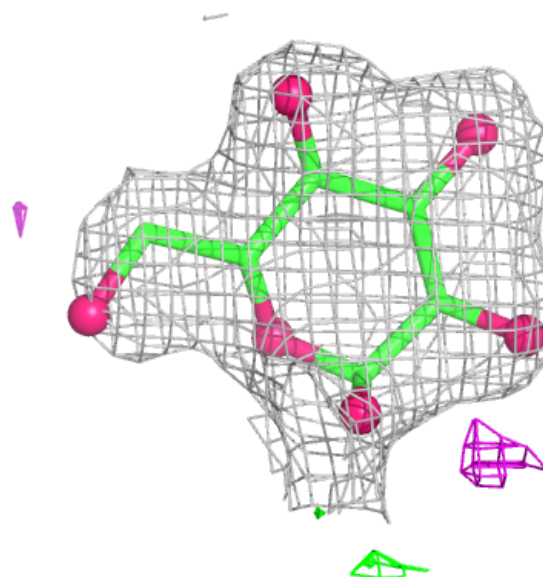
Electron density around GLC M 506:

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



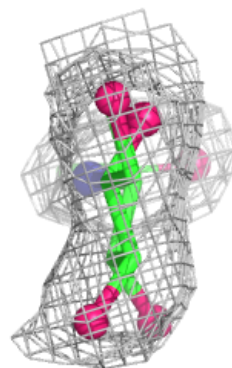
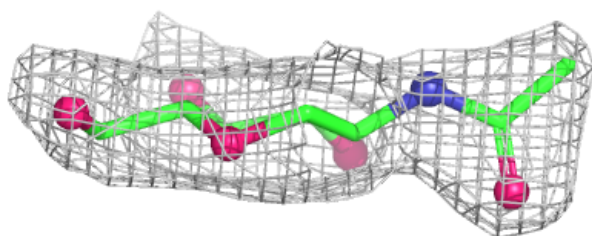
Electron density around GLC P 1002:

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

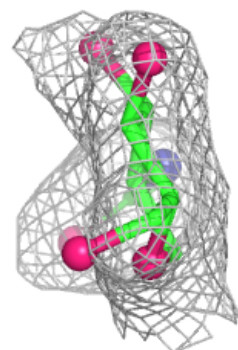
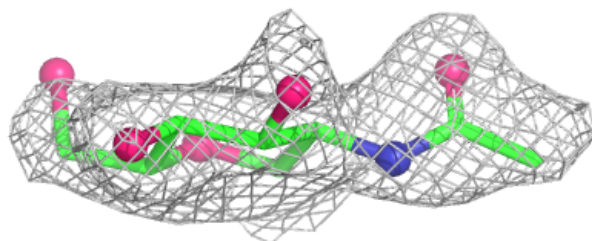
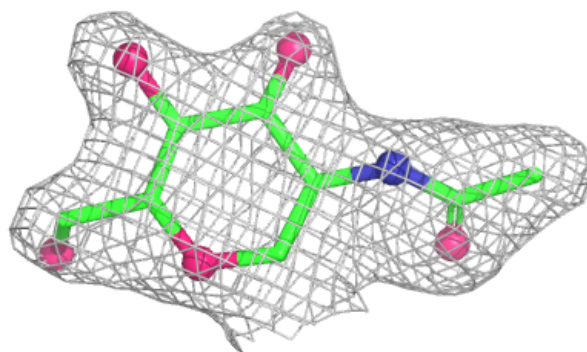


Electron density around NAG D 1002:

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

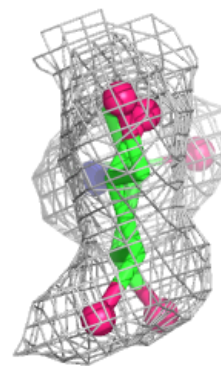
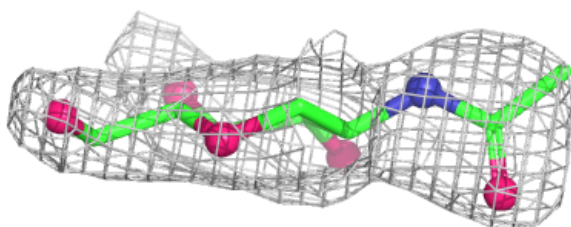
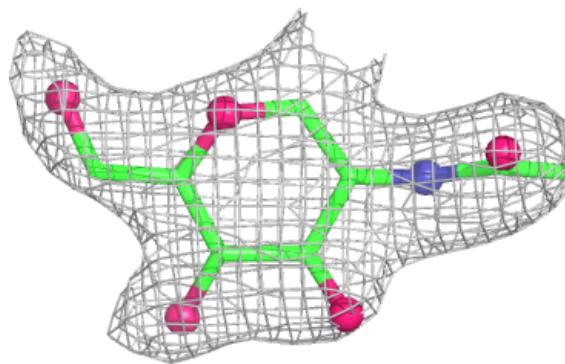
**Electron density around NAG O 505:**

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

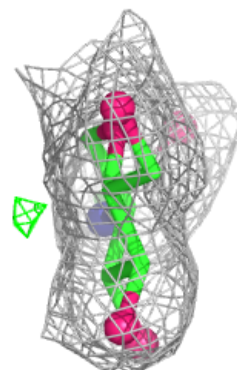
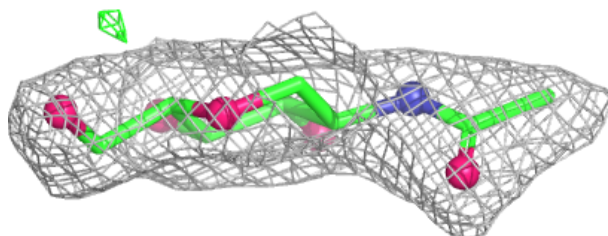
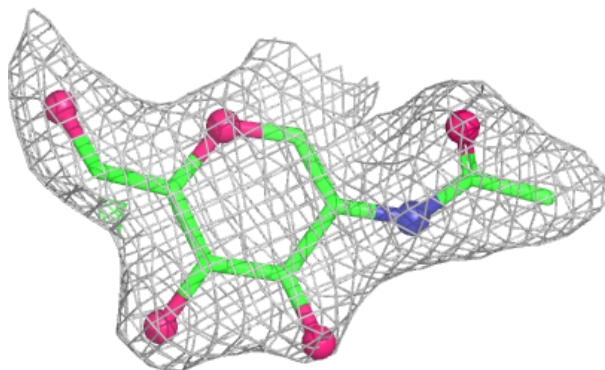


Electron density around NAG P 1003:

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

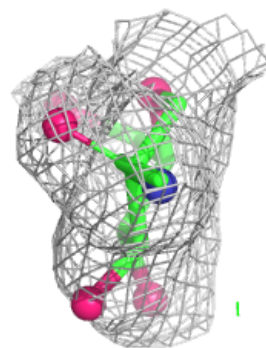
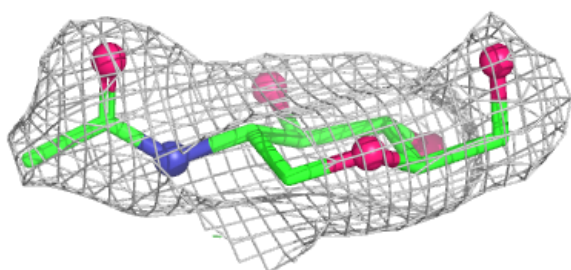
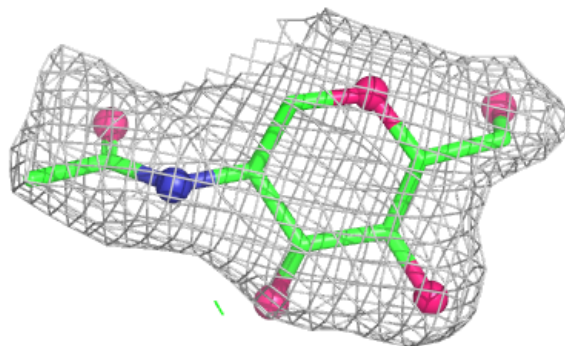
**Electron density around NAG A 505:**

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

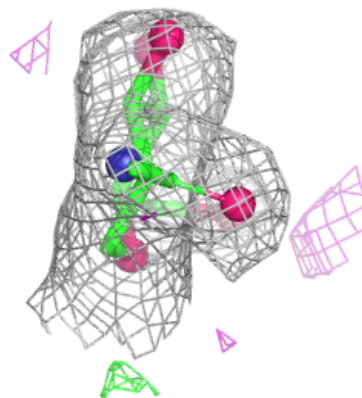
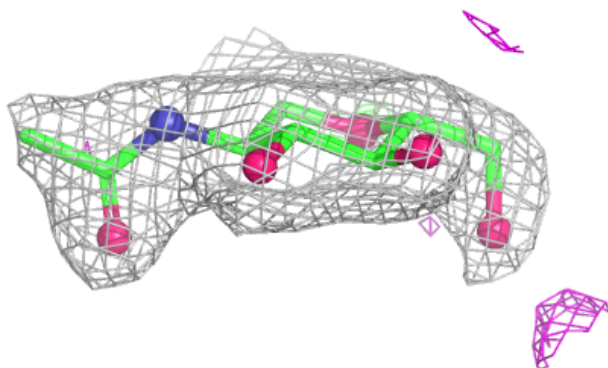
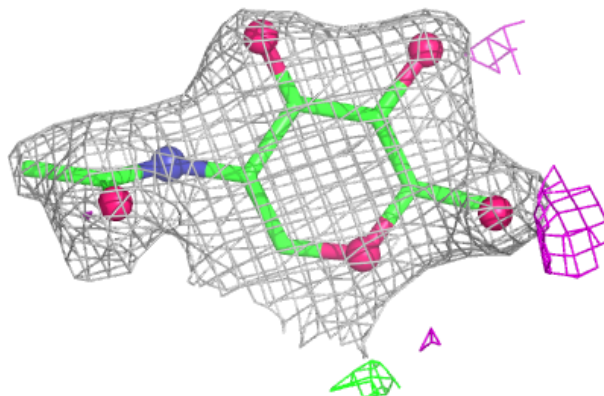


Electron density around NAG G 504:

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

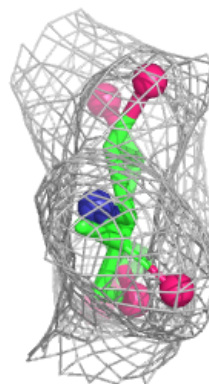
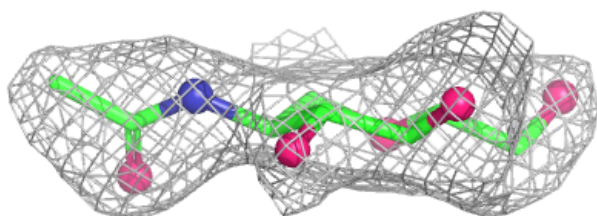
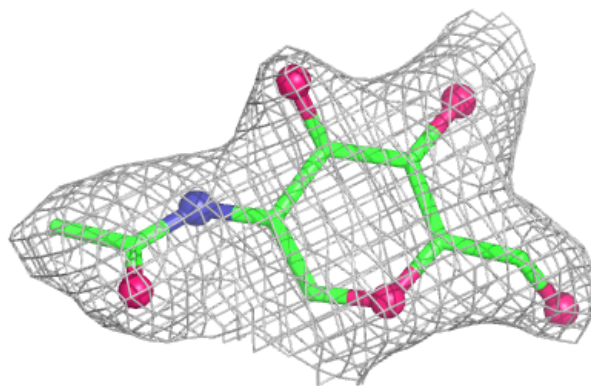
**Electron density around NAG I 504:**

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



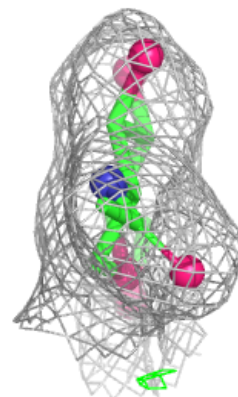
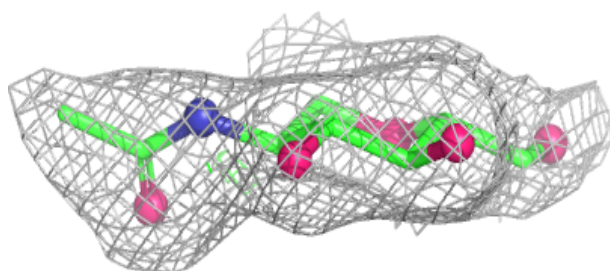
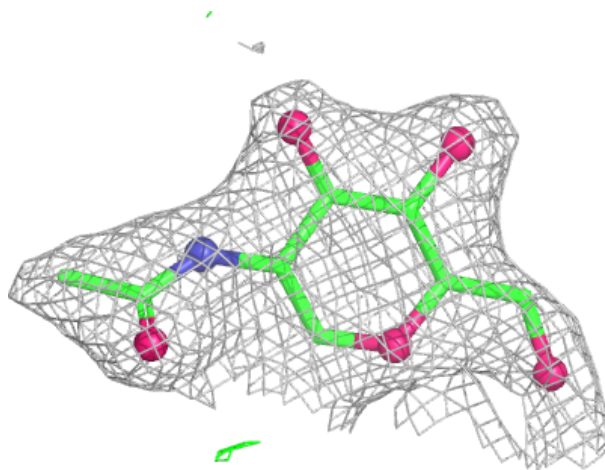
Electron density around NAG I 505:

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



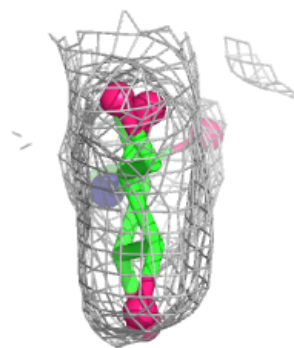
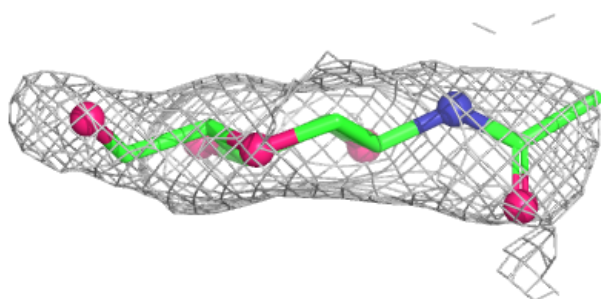
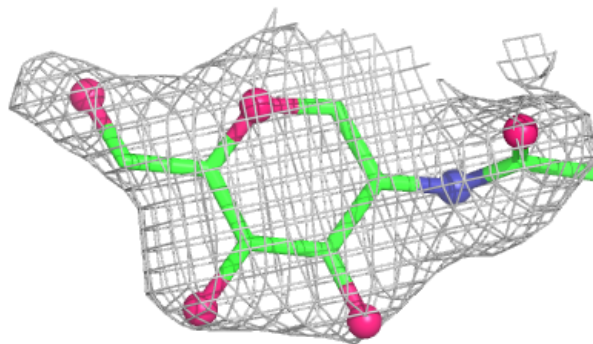
Electron density around NAG M 505:

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

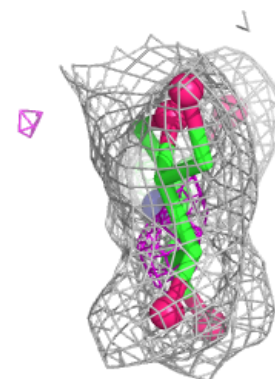
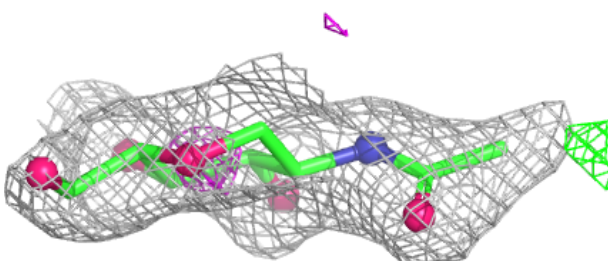
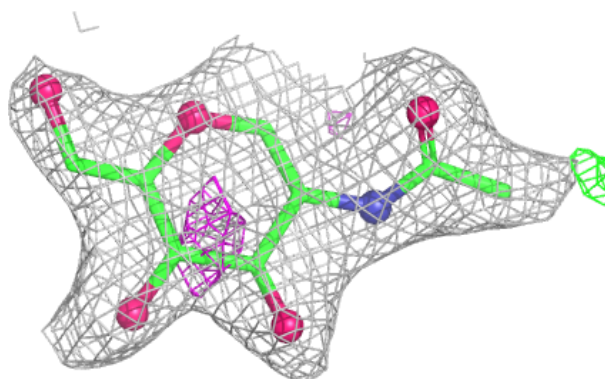


Electron density around NAG J 1003:

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

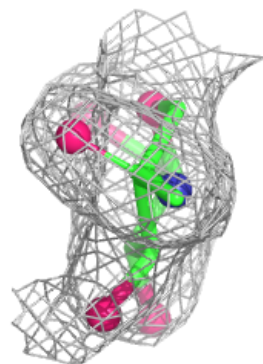
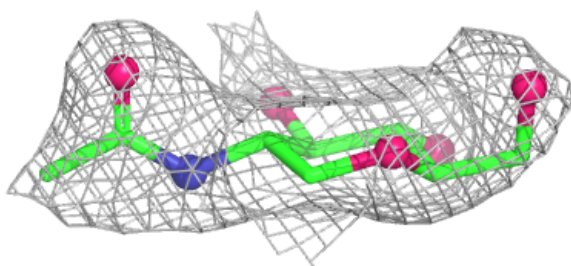
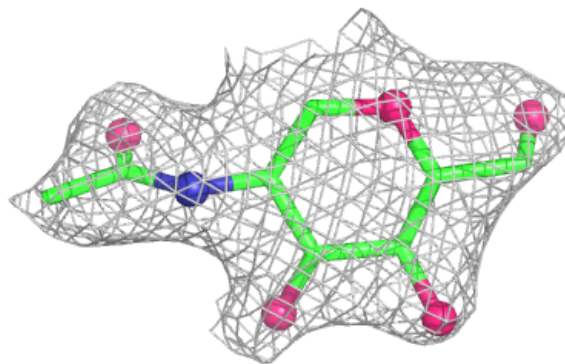
**Electron density around NAG G 505:**

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

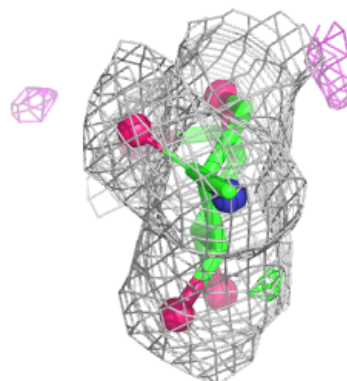
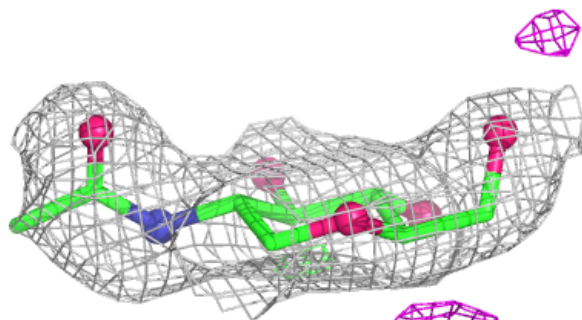
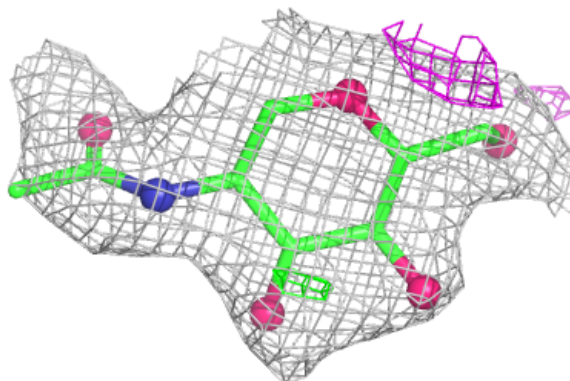


Electron density around NAG O 502:

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

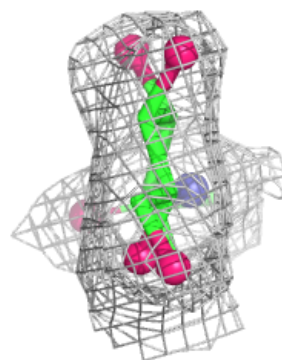
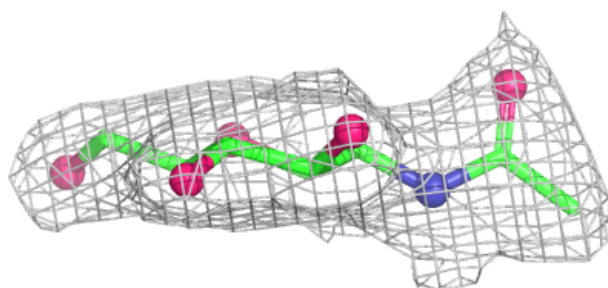
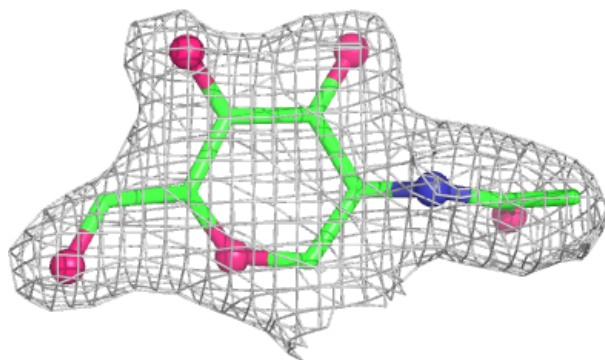
**Electron density around NAG A 504:**

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

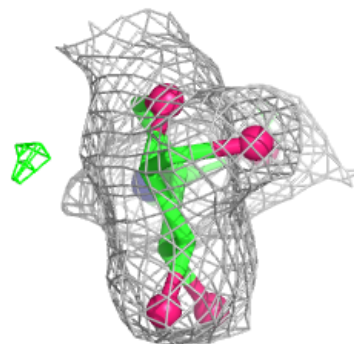
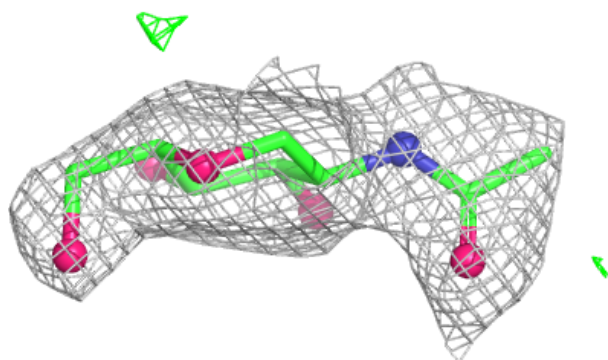
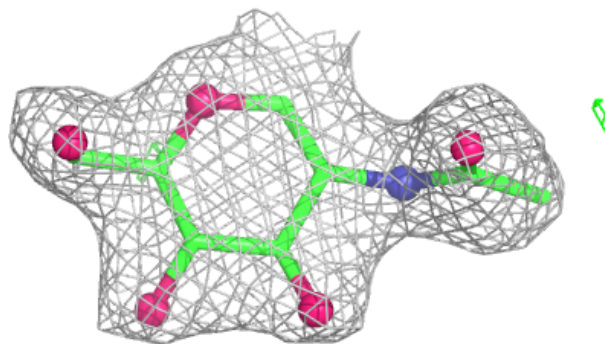


Electron density around NAG H 1002:

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

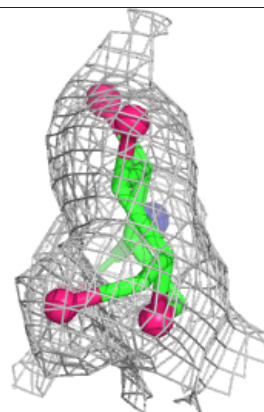
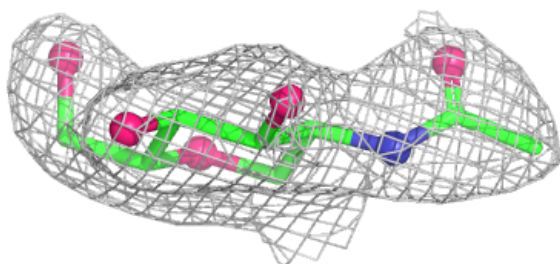
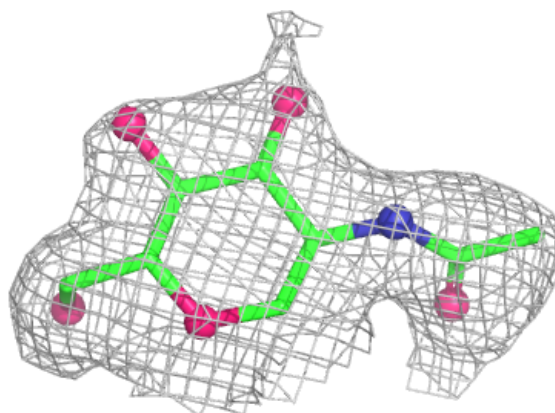
**Electron density around NAG K 501:**

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

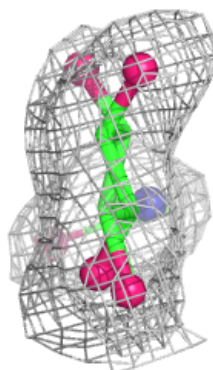
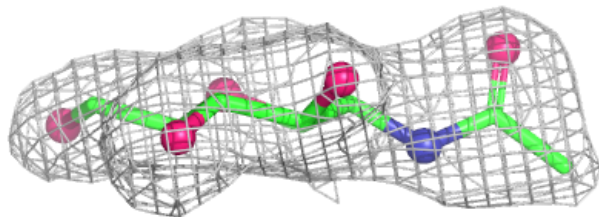
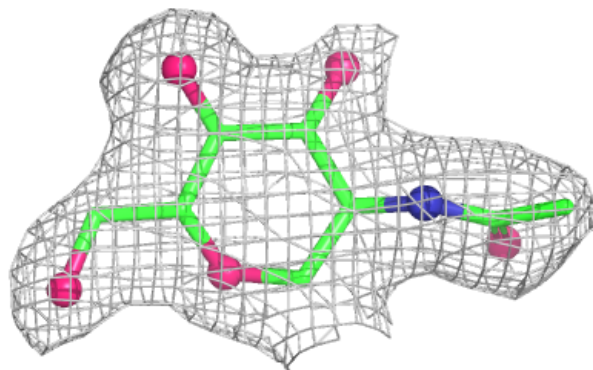


Electron density around NAG K 502:

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

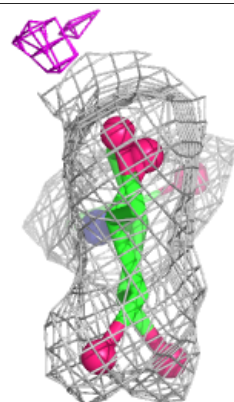
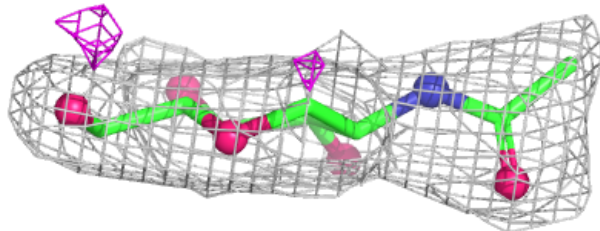
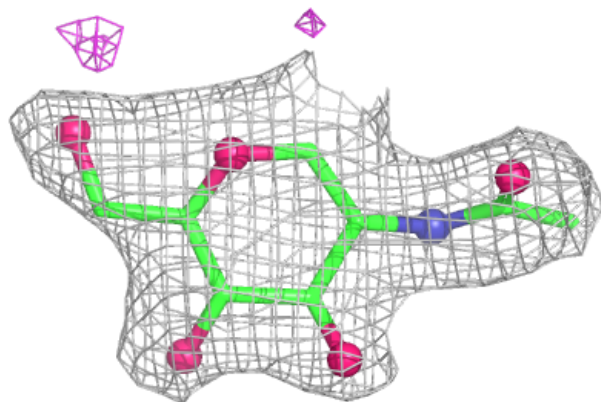
**Electron density around NAG F 1002:**

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

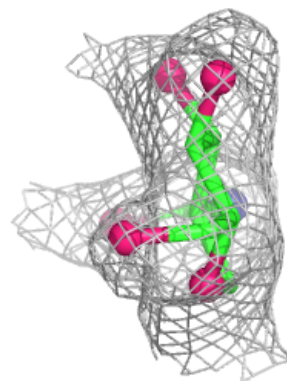
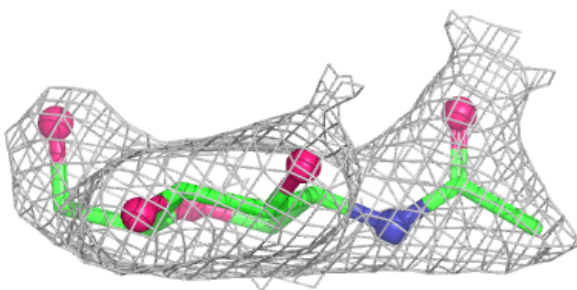
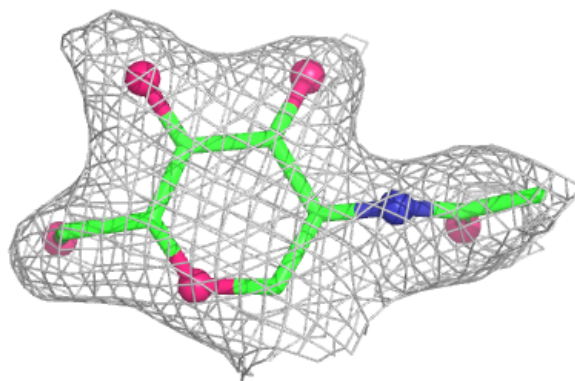


Electron density around NAG L 1003:

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

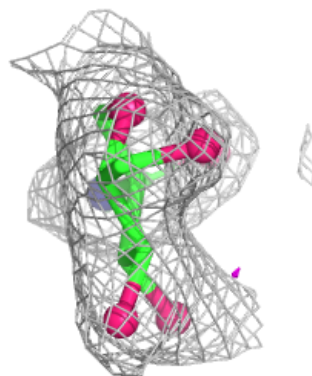
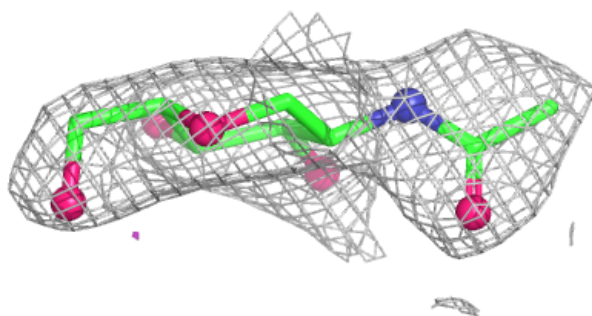
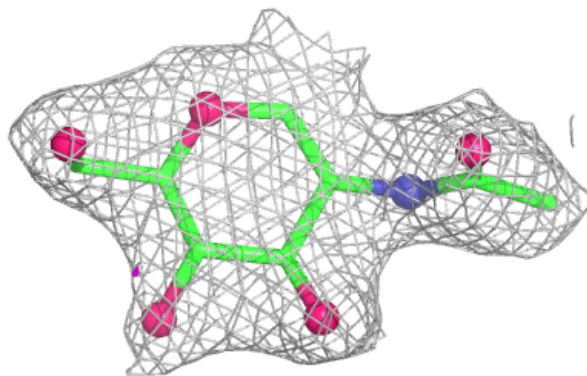
**Electron density around NAG C 502:**

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

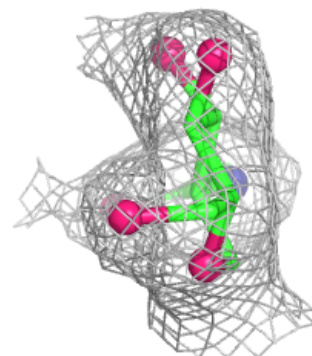
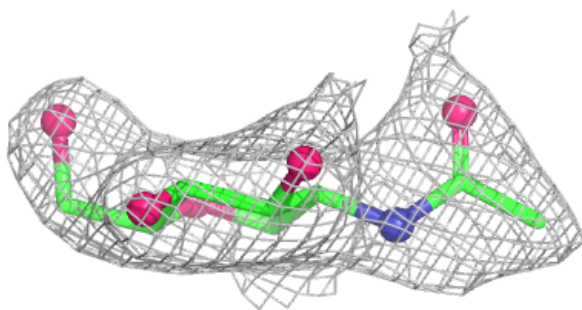
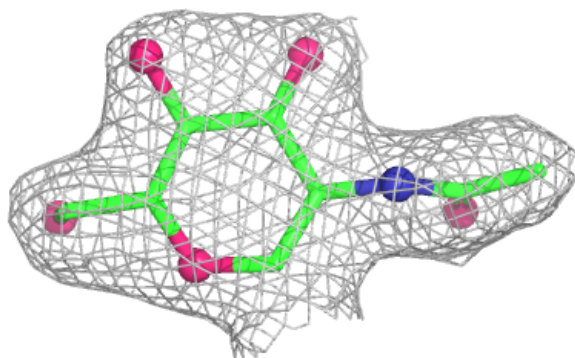


Electron density around NAG E 502:

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

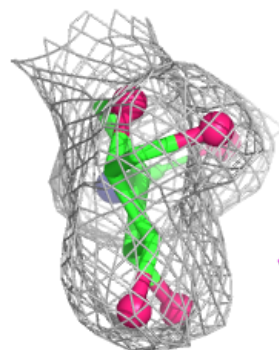
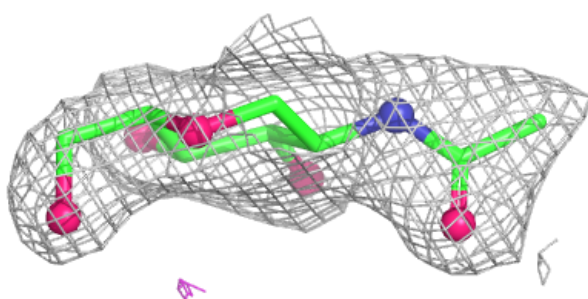
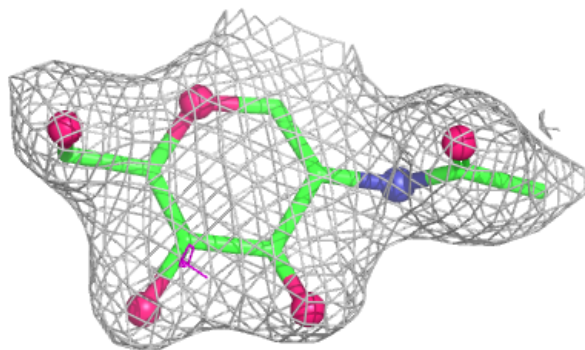
**Electron density around NAG I 502:**

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

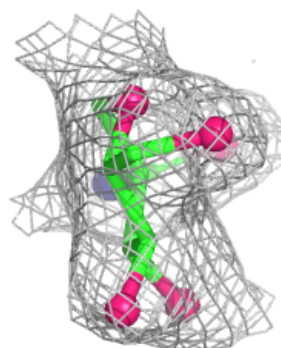
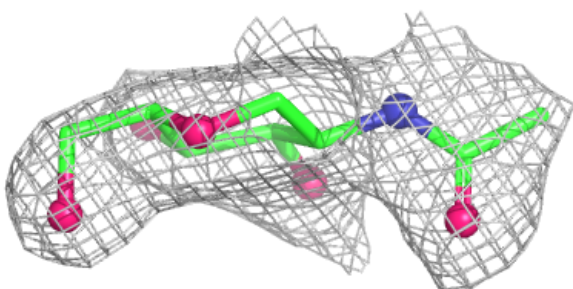
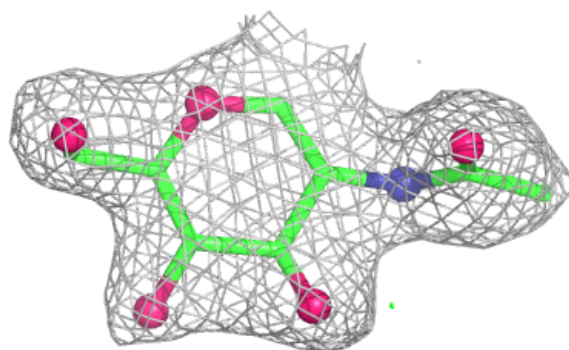


Electron density around NAG G 502:

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

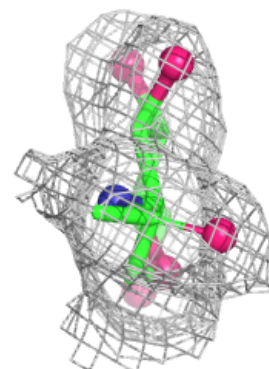
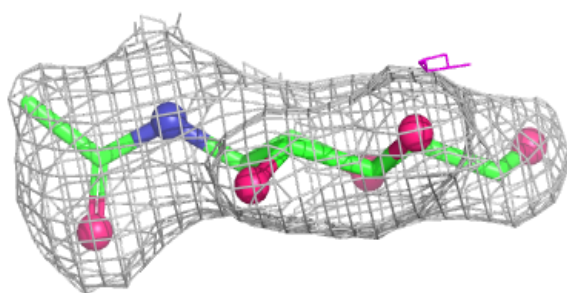
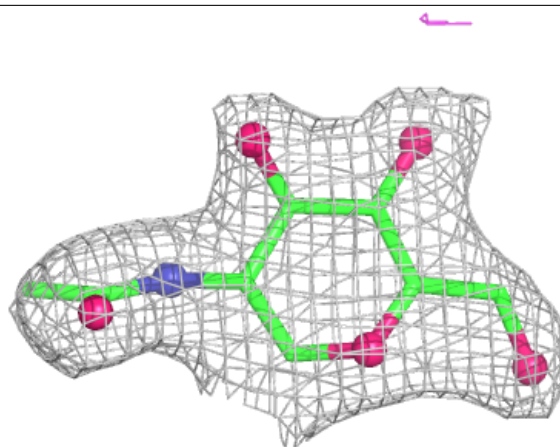
**Electron density around NAG A 502:**

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



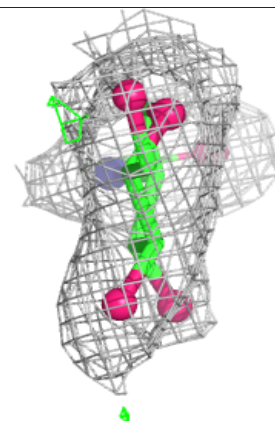
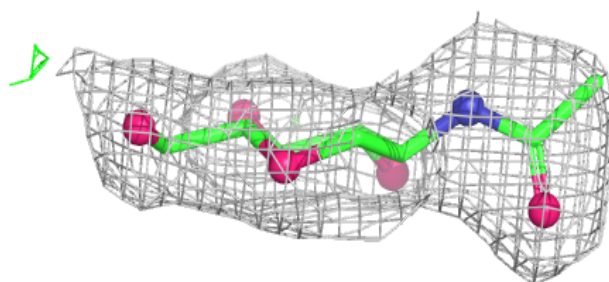
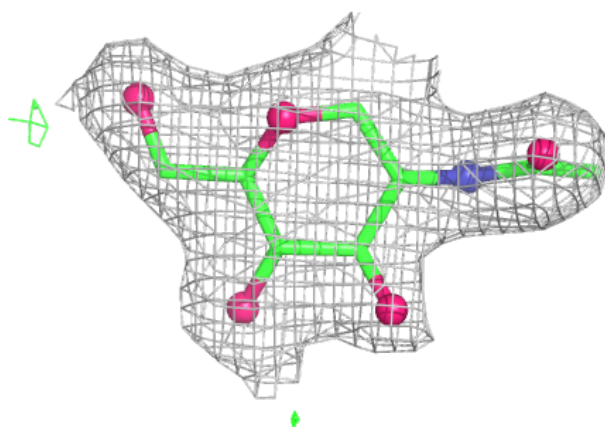
Electron density around NAG B 1003:

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

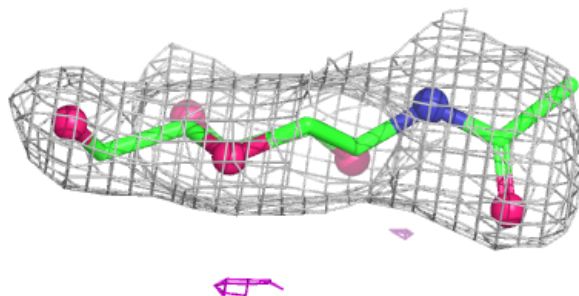


Electron density around NAG N 1002:

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

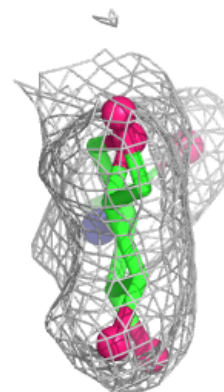
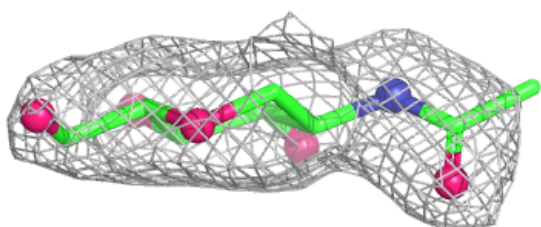
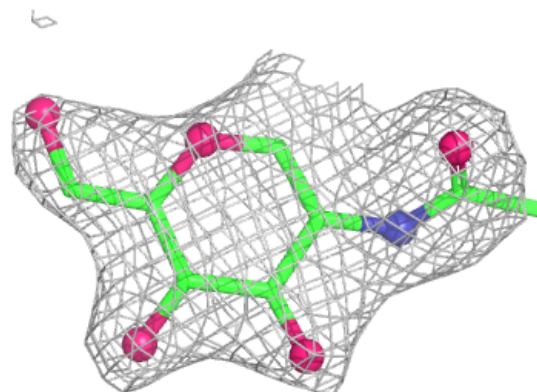
**Electron density around NAG J 1002:**

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

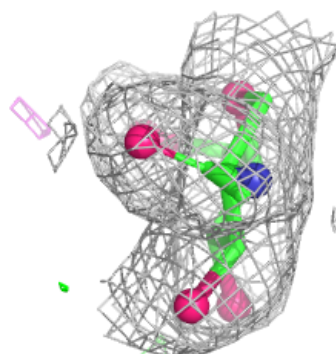
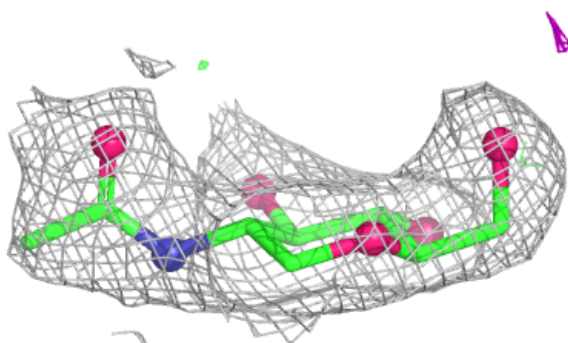
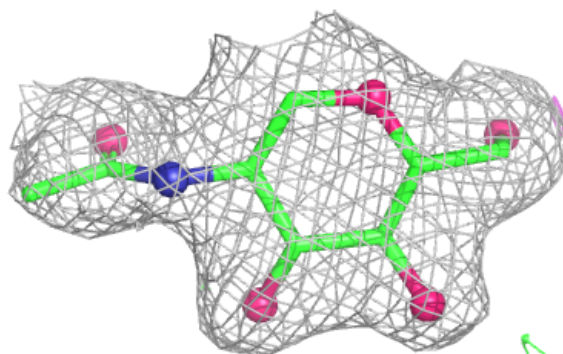


Electron density around NAG E 505:

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

**Electron density around NAG M 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.