



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 22, 2025 – 01:58 AM EDT

PDB ID : 8TDH / pdb\_00008tdh  
Title : Structure of trehalose bound Alistipes sp. Glucoside-3-dehydrogenase AL3  
Authors : Lazarski, A.C.; Worrall, L.J.; Strynadka, N.C.J.  
Deposited on : 2023-07-03  
Resolution : 2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

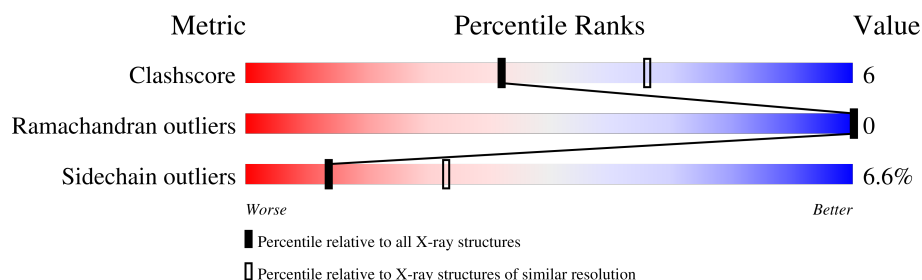
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
Clashscore	180529	1097 (2.98-2.94)
Ramachandran outliers	177936	1049 (2.98-2.94)
Sidechain outliers	177891	1049 (2.98-2.94)



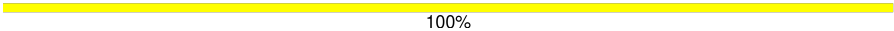

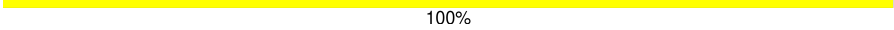


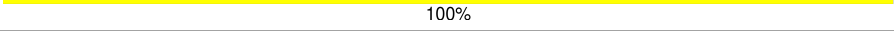
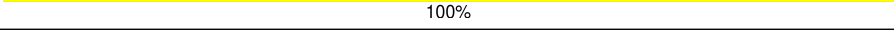
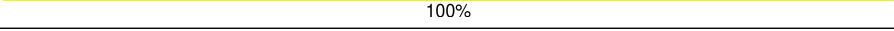
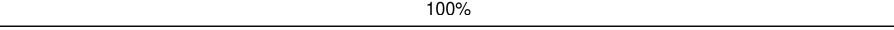

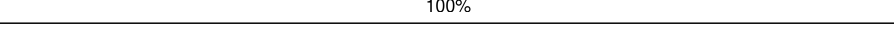
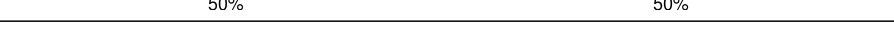



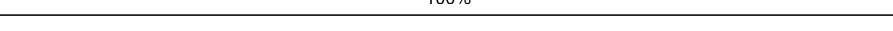
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	451	78% 19% .
1	B	451	81% 17% .
1	C	451	82% 16% .
1	D	451	78% 18% .
2	E	2	100%
2	G	2	100%
2	H	2	100%
2	L	2	100%

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Mol	Chain	Length	Quality of chain
2	P	2	 50% 50%
2	Q	2	 50% 50%
2	T	2	 100%
2	U	2	 100%
2	V	2	 100%
2	W	2	 100%
3	F	2	 50% 50%
3	I	2	 100%
3	J	2	 100%
3	K	2	 100%
3	M	2	 100%
3	N	2	 50% 50%
3	O	2	 100%
3	R	2	 50% 50%
3	S	2	 50% 50%
3	X	2	 50% 50%
3	Y	2	 50% 50%
3	Z	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	W	2	-	-	X	-

## 2 Entry composition [i](#)

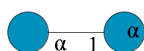
There are 5 unique types of molecules in this entry. The entry contains 15008 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Predicted dehydrogenases and related proteins.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3531	2255	609	646	21			
1	B	451	Total	C	N	O	S	0	0	0
			3559	2271	617	650	21			
1	C	451	Total	C	N	O	S	0	0	0
			3559	2271	617	650	21			
1	D	451	Total	C	N	O	S	0	0	0
			3559	2271	617	650	21			

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			
2	P	2	Total	C	O	0	0	0
			23	12	11			
2	Q	2	Total	C	O	0	0	0
			23	12	11			
2	T	2	Total	C	O	0	0	0
			23	12	11			
2	U	2	Total	C	O	0	0	0
			23	12	11			

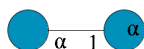
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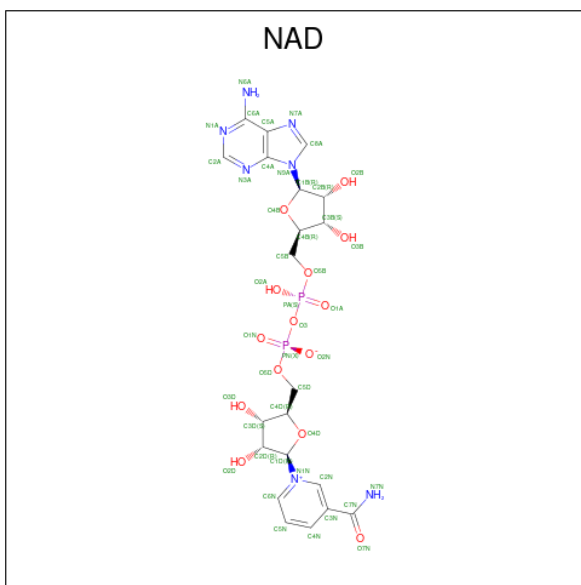
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	V	2	Total	C	O	0	0	0
			23	12	11			
2	W	2	Total	C	O	0	0	0
			23	12	11			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	F	2	Total	C	O	0	0	0
			23	12	11			
3	I	2	Total	C	O	0	0	0
			23	12	11			
3	J	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	N	2	Total	C	O	0	0	0
			23	12	11			
3	O	2	Total	C	O	0	0	0
			23	12	11			
3	R	2	Total	C	O	0	0	0
			23	12	11			
3	S	2	Total	C	O	0	0	0
			23	12	11			
3	X	2	Total	C	O	0	0	0
			23	12	11			
3	Y	2	Total	C	O	0	0	0
			23	12	11			
3	Z	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 5 is water.

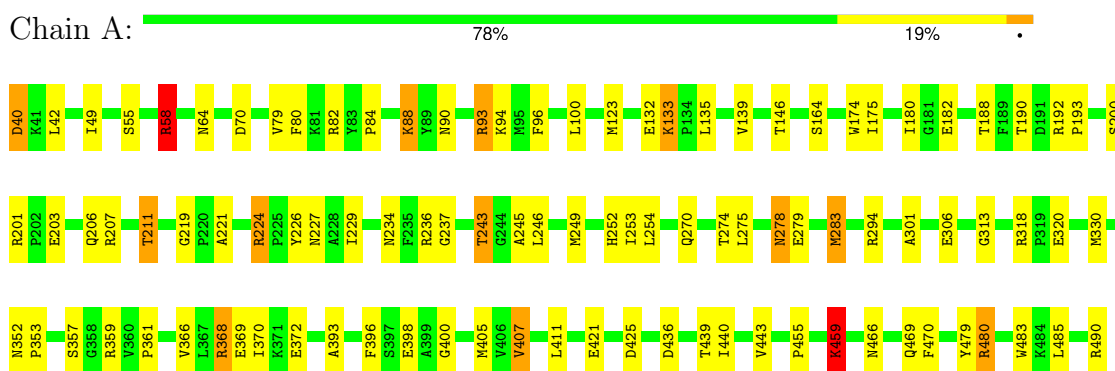
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	41	Total O 41 41	0	0
5	B	30	Total O 30 30	0	0
5	C	25	Total O 25 25	0	0
5	D	22	Total O 22 22	0	0

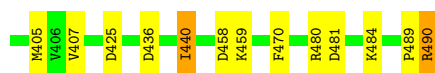
### 3 Residue-property plots

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. 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. 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.

Note EDS failed to run properly.

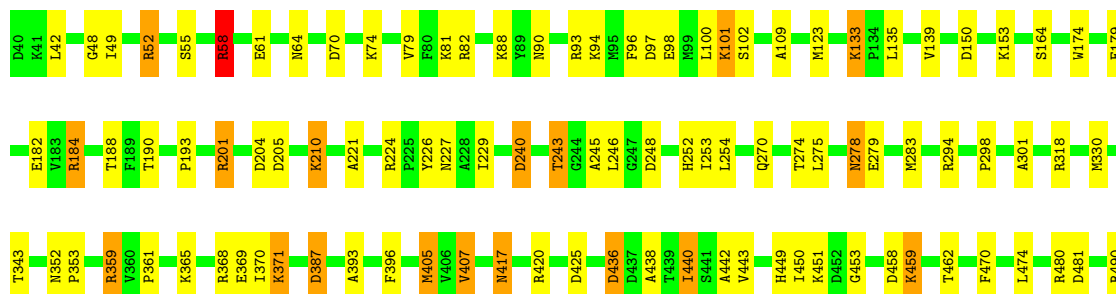
- Molecule 1: Predicted dehydrogenases and related proteins





- Molecule 1: Predicted dehydrogenases and related proteins

Chain D: 78% 18%



- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain E: 100%



- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain G: 100%



- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain H: 100%



- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain L: 100%



- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain P: 50% 50%



- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain Q:  50% 50%

GLC1  
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain T:  100%

GLC1  
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain U:  100%

GLC1  
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain V:  100%

GLC1  
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain W:  100%

GLC1  
GLC2

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

Chain F:  50% 50%

GLC1  
GLC2

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

Chain I:  100%

GLC1  
GLC2

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

Chain J:  100%

GLC1  
GLC2

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

Chain K:  100%GLC1  
GLC2

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

Chain M:  100%GLC1  
GLC2

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

Chain N:  50% 50%GLC1  
GLC2

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

Chain O:  100%GLC1  
GLC2

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

Chain R:  50% 50%GLC1  
GLC2


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

Chain S:  50% 50%GLC1  
GLC2

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

Chain X:  50% 50%GLC1  
GLC2

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

Chain Y:  50% 50%

GLC1  
GLC2

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

Chain Z:  100%

GLC1  
GLC2

## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.58Å 57.22Å 224.96Å 90.00° 106.58° 90.00°	Depositor
Resolution (Å)	162.27 – 2.95	Depositor
% Data completeness (in resolution range)	89.7 (162.27-2.95)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.195 , 0.247	Depositor
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.088	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAD, GLC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.70	6/3630 (0.2%)	1.17	25/4938 (0.5%)
1	B	0.61	1/3658 (0.0%)	1.07	11/4969 (0.2%)
1	C	0.58	1/3658 (0.0%)	1.10	15/4969 (0.3%)
1	D	0.54	1/3658 (0.0%)	1.06	15/4969 (0.3%)
All	All	0.61	9/14604 (0.1%)	1.10	66/19845 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	2
1	C	0	5
1	D	0	7
All	All	0	19

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	GLU	CD-OE1	7.13	1.33	1.25
1	A	398	GLU	CD-OE1	7.08	1.33	1.25
1	A	306	GLU	CD-OE2	6.93	1.33	1.25
1	A	369	GLU	CD-OE2	6.29	1.32	1.25
1	A	306	GLU	CD-OE1	6.22	1.32	1.25

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	283	MET	CG-SD-CE	14.71	123.74	100.20
1	A	224	ARG	NE-CZ-NH1	-10.68	114.96	120.30
1	A	405	MET	CG-SD-CE	10.05	116.28	100.20
1	A	207	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	D	52	ARG	NE-CZ-NH1	-8.66	115.97	120.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	368	ARG	Sidechain
1	A	40	ASP	Peptide
1	A	58	ARG	Sidechain
1	A	93	ARG	Sidechain

## 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	3531	0	3426	47	0
1	B	3559	0	3488	50	0
1	C	3559	0	3488	34	0
1	D	3559	0	3488	54	0
2	E	23	0	21	1	0
2	G	23	0	21	2	0
2	H	23	0	21	0	0
2	L	23	0	21	0	0
2	P	23	0	21	1	0
2	Q	23	0	21	1	0
2	T	23	0	21	0	0
2	U	23	0	21	4	0
2	V	23	0	21	0	0
2	W	23	0	21	7	0
3	F	23	0	21	3	0
3	I	23	0	21	0	0
3	J	23	0	21	0	0
3	K	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	23	0	21	0	0
3	N	23	0	21	1	0
3	O	23	0	21	0	0
3	R	23	0	21	1	0
3	S	23	0	21	2	0
3	X	23	0	21	0	0
3	Y	23	0	21	3	0
3	Z	23	0	21	0	0
4	A	44	0	26	3	0
4	B	44	0	26	3	0
4	C	44	0	26	2	0
4	D	44	0	26	2	0
5	A	41	0	0	5	0
5	B	30	0	0	4	0
5	C	25	0	0	1	0
5	D	22	0	0	2	0
All	All	15008	0	14456	183	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 183 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:HB2	3:Y:1:GLC:H61	1.41	1.02
1:D:462:THR:HG21	2:W:2:GLC:O6	1.67	0.94
2:G:1:GLC:H5	2:G:2:GLC:H1	1.49	0.93
1:D:184:ARG:HB2	3:S:1:GLC:H61	1.58	0.83
1:B:201:ARG:NH1	1:B:279:GLU:OE2	2.14	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	449/451 (100%)	427 (95%)	22 (5%)	0	100	100
1	B	449/451 (100%)	430 (96%)	19 (4%)	0	100	100
1	C	449/451 (100%)	429 (96%)	20 (4%)	0	100	100
1	D	449/451 (100%)	433 (96%)	16 (4%)	0	100	100
All	All	1796/1804 (100%)	1719 (96%)	77 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	367/375 (98%)	349 (95%)	18 (5%)	21	45
1	B	375/375 (100%)	352 (94%)	23 (6%)	15	36
1	C	375/375 (100%)	347 (92%)	28 (8%)	11	27
1	D	375/375 (100%)	345 (92%)	30 (8%)	10	25
All	All	1492/1500 (100%)	1393 (93%)	99 (7%)	14	33

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	278	ASN
1	D	64	ASN
1	C	298	PRO
1	C	459	LYS
1	D	97	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	477	HIS
1	D	278	ASN
1	D	477	HIS
1	D	469	GLN
1	B	252	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

44 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GLC	E	1	2	11,11,12	1.21	1 (9%)	15,15,17	2.96	3 (20%)
2	GLC	E	2	2	12,12,12	0.78	0	17,17,17	1.24	2 (11%)
3	GLC	F	1	3	12,12,12	0.60	0	17,17,17	1.35	3 (17%)
3	GLC	F	2	3	11,11,12	1.30	1 (9%)	15,15,17	2.30	7 (46%)
2	GLC	G	1	2	11,11,12	1.08	1 (9%)	15,15,17	1.45	2 (13%)
2	GLC	G	2	2	12,12,12	1.03	1 (8%)	17,17,17	1.87	4 (23%)
2	GLC	H	1	2	11,11,12	0.93	0	15,15,17	2.57	2 (13%)
2	GLC	H	2	2	12,12,12	0.98	1 (8%)	17,17,17	2.03	5 (29%)
3	GLC	I	1	3	12,12,12	0.61	0	17,17,17	1.25	2 (11%)
3	GLC	I	2	3	11,11,12	0.80	0	15,15,17	2.20	4 (26%)
3	GLC	J	1	3	12,12,12	0.76	0	17,17,17	1.75	3 (17%)
3	GLC	J	2	3	11,11,12	0.61	0	15,15,17	1.73	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLC	K	1	3	12,12,12	0.74	0	17,17,17	1.60	5 (29%)
3	GLC	K	2	3	11,11,12	1.01	1 (9%)	15,15,17	1.52	2 (13%)
2	GLC	L	1	2	11,11,12	0.84	0	15,15,17	1.61	5 (33%)
2	GLC	L	2	2	12,12,12	0.53	0	17,17,17	1.80	3 (17%)
3	GLC	M	1	3	12,12,12	0.96	1 (8%)	17,17,17	1.53	4 (23%)
3	GLC	M	2	3	11,11,12	0.59	0	15,15,17	1.32	2 (13%)
3	GLC	N	1	3	12,12,12	0.88	0	17,17,17	1.64	6 (35%)
3	GLC	N	2	3	11,11,12	0.95	0	15,15,17	3.54	7 (46%)
3	GLC	O	1	3	12,12,12	0.48	0	17,17,17	1.78	4 (23%)
3	GLC	O	2	3	11,11,12	0.66	0	15,15,17	3.28	4 (26%)
2	GLC	P	1	2	11,11,12	0.72	0	15,15,17	1.87	5 (33%)
2	GLC	P	2	2	12,12,12	0.74	0	17,17,17	1.10	1 (5%)
2	GLC	Q	1	2	11,11,12	0.96	1 (9%)	15,15,17	1.78	4 (26%)
2	GLC	Q	2	2	12,12,12	0.45	0	17,17,17	1.23	2 (11%)
3	GLC	R	1	3	12,12,12	0.46	0	17,17,17	1.52	5 (29%)
3	GLC	R	2	3	11,11,12	0.59	0	15,15,17	2.33	6 (40%)
3	GLC	S	1	3	12,12,12	0.54	0	17,17,17	1.43	5 (29%)
3	GLC	S	2	3	11,11,12	0.55	0	15,15,17	1.34	2 (13%)
2	GLC	T	1	2	11,11,12	0.77	0	15,15,17	1.77	4 (26%)
2	GLC	T	2	2	12,12,12	1.45	1 (8%)	17,17,17	2.03	4 (23%)
2	GLC	U	1	2	11,11,12	1.40	2 (18%)	15,15,17	1.95	3 (20%)
2	GLC	U	2	2	12,12,12	0.94	1 (8%)	17,17,17	1.38	1 (5%)
2	GLC	V	1	2	11,11,12	0.92	1 (9%)	15,15,17	1.47	3 (20%)
2	GLC	V	2	2	12,12,12	0.47	0	17,17,17	1.86	5 (29%)
2	GLC	W	1	2	11,11,12	1.42	2 (18%)	15,15,17	2.76	5 (33%)
2	GLC	W	2	2	12,12,12	0.81	0	17,17,17	1.52	4 (23%)
3	GLC	X	1	3	12,12,12	0.38	0	17,17,17	0.89	0
3	GLC	X	2	3	11,11,12	1.09	1 (9%)	15,15,17	1.73	3 (20%)
3	GLC	Y	1	3	12,12,12	0.33	0	17,17,17	1.23	1 (5%)
3	GLC	Y	2	3	11,11,12	0.56	0	15,15,17	1.93	5 (33%)
3	GLC	Z	1	3	12,12,12	0.66	0	17,17,17	1.38	2 (11%)
3	GLC	Z	2	3	11,11,12	0.74	0	15,15,17	2.03	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	E	1	2	-	2/2/19/22	0/1/1/1
2	GLC	E	2	2	-	2/2/22/22	0/1/1/1
3	GLC	F	1	3	-	2/2/22/22	0/1/1/1
3	GLC	F	2	3	-	2/2/19/22	0/1/1/1
2	GLC	G	1	2	-	2/2/19/22	0/1/1/1
2	GLC	G	2	2	-	0/2/22/22	0/1/1/1
2	GLC	H	1	2	-	2/2/19/22	0/1/1/1
2	GLC	H	2	2	-	2/2/22/22	0/1/1/1
3	GLC	I	1	3	-	2/2/22/22	0/1/1/1
3	GLC	I	2	3	-	0/2/19/22	0/1/1/1
3	GLC	J	1	3	-	0/2/22/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	K	1	3	-	2/2/22/22	0/1/1/1
3	GLC	K	2	3	-	0/2/19/22	0/1/1/1
2	GLC	L	1	2	-	2/2/19/22	0/1/1/1
2	GLC	L	2	2	-	0/2/22/22	0/1/1/1
3	GLC	M	1	3	-	0/2/22/22	0/1/1/1
3	GLC	M	2	3	-	2/2/19/22	0/1/1/1
3	GLC	N	1	3	-	0/2/22/22	0/1/1/1
3	GLC	N	2	3	-	2/2/19/22	0/1/1/1
3	GLC	O	1	3	-	2/2/22/22	0/1/1/1
3	GLC	O	2	3	-	1/2/19/22	0/1/1/1
2	GLC	P	1	2	-	2/2/19/22	0/1/1/1
2	GLC	P	2	2	-	2/2/22/22	0/1/1/1
2	GLC	Q	1	2	-	2/2/19/22	0/1/1/1
2	GLC	Q	2	2	-	0/2/22/22	0/1/1/1
3	GLC	R	1	3	-	0/2/22/22	0/1/1/1
3	GLC	R	2	3	-	2/2/19/22	0/1/1/1
3	GLC	S	1	3	-	2/2/22/22	0/1/1/1
3	GLC	S	2	3	-	2/2/19/22	0/1/1/1
2	GLC	T	1	2	-	0/2/19/22	0/1/1/1
2	GLC	T	2	2	-	2/2/22/22	0/1/1/1
2	GLC	U	1	2	-	2/2/19/22	0/1/1/1
2	GLC	U	2	2	-	2/2/22/22	0/1/1/1
2	GLC	V	1	2	-	2/2/19/22	0/1/1/1
2	GLC	V	2	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	W	1	2	-	2/2/19/22	0/1/1/1
2	GLC	W	2	2	-	2/2/22/22	0/1/1/1
3	GLC	X	1	3	-	0/2/22/22	0/1/1/1
3	GLC	X	2	3	-	2/2/19/22	0/1/1/1
3	GLC	Y	1	3	-	2/2/22/22	0/1/1/1
3	GLC	Y	2	3	-	1/2/19/22	0/1/1/1
3	GLC	Z	1	3	-	0/2/22/22	0/1/1/1
3	GLC	Z	2	3	-	2/2/19/22	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	2	GLC	C4-C5	4.34	1.62	1.53
3	F	2	GLC	C4-C5	3.84	1.61	1.53
2	Q	1	GLC	C1-C2	2.85	1.59	1.52
2	U	1	GLC	C4-C5	2.82	1.59	1.53
3	X	2	GLC	C4-C5	2.69	1.58	1.53

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	2	GLC	C1-O5-C5	11.02	126.96	112.19
3	N	2	GLC	C1-O5-C5	9.79	125.31	112.19
2	H	1	GLC	C1-O5-C5	8.46	123.53	112.19
2	E	1	GLC	C1-C2-C3	7.67	120.81	109.64
2	E	1	GLC	C1-O5-C5	-7.09	102.69	112.19

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	W	2	GLC	O5-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
3	O	1	GLC	O5-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	Q	1	GLC	C4-C5-C6-O6

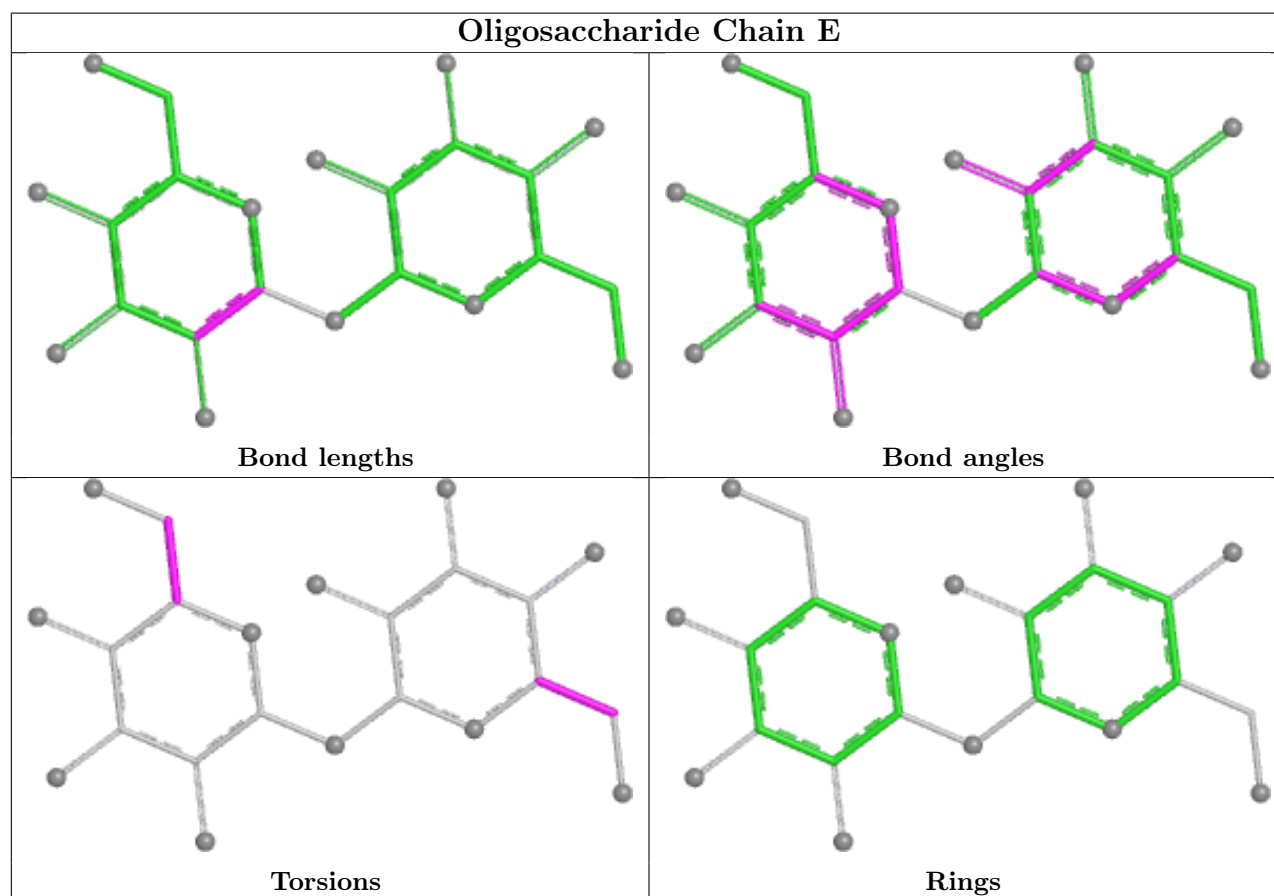
There are no ring outliers.

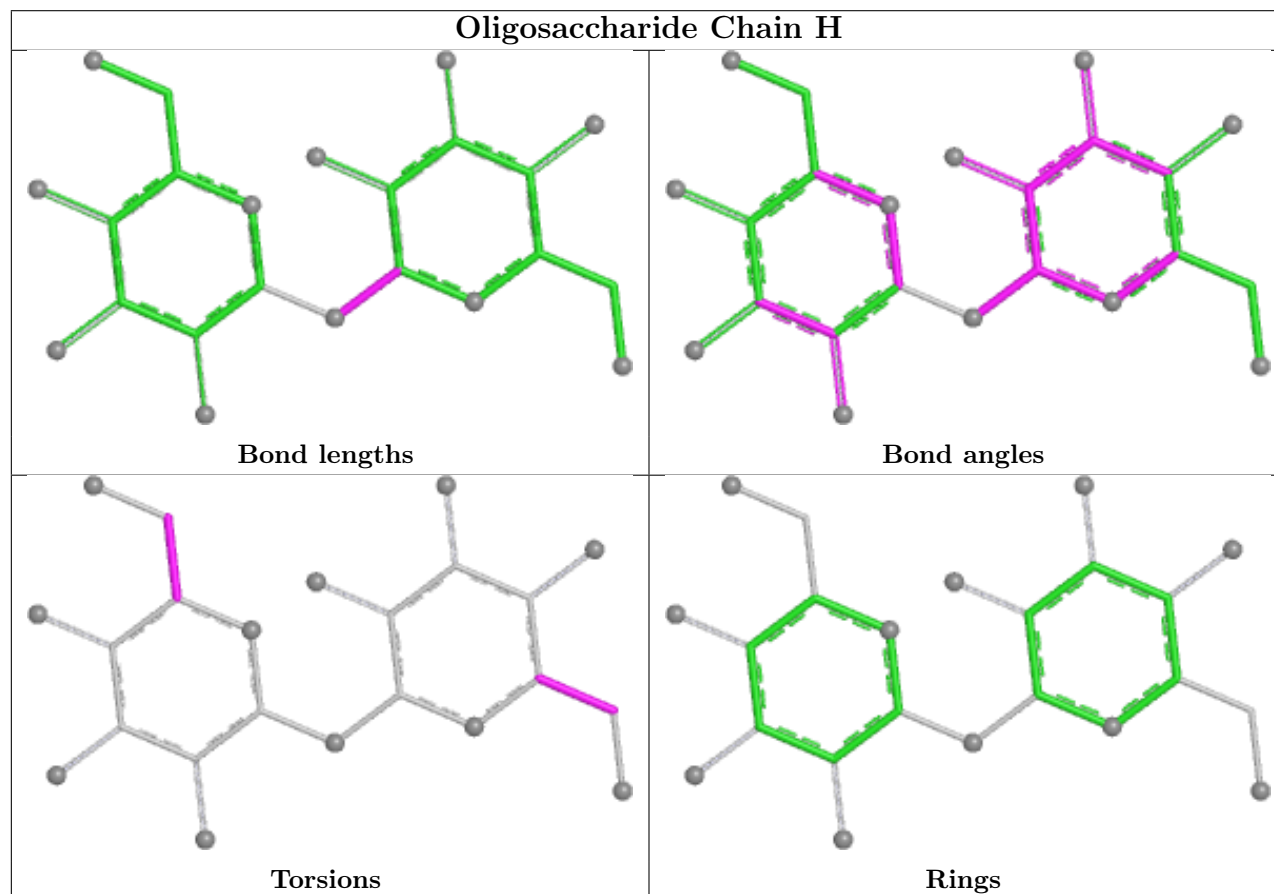
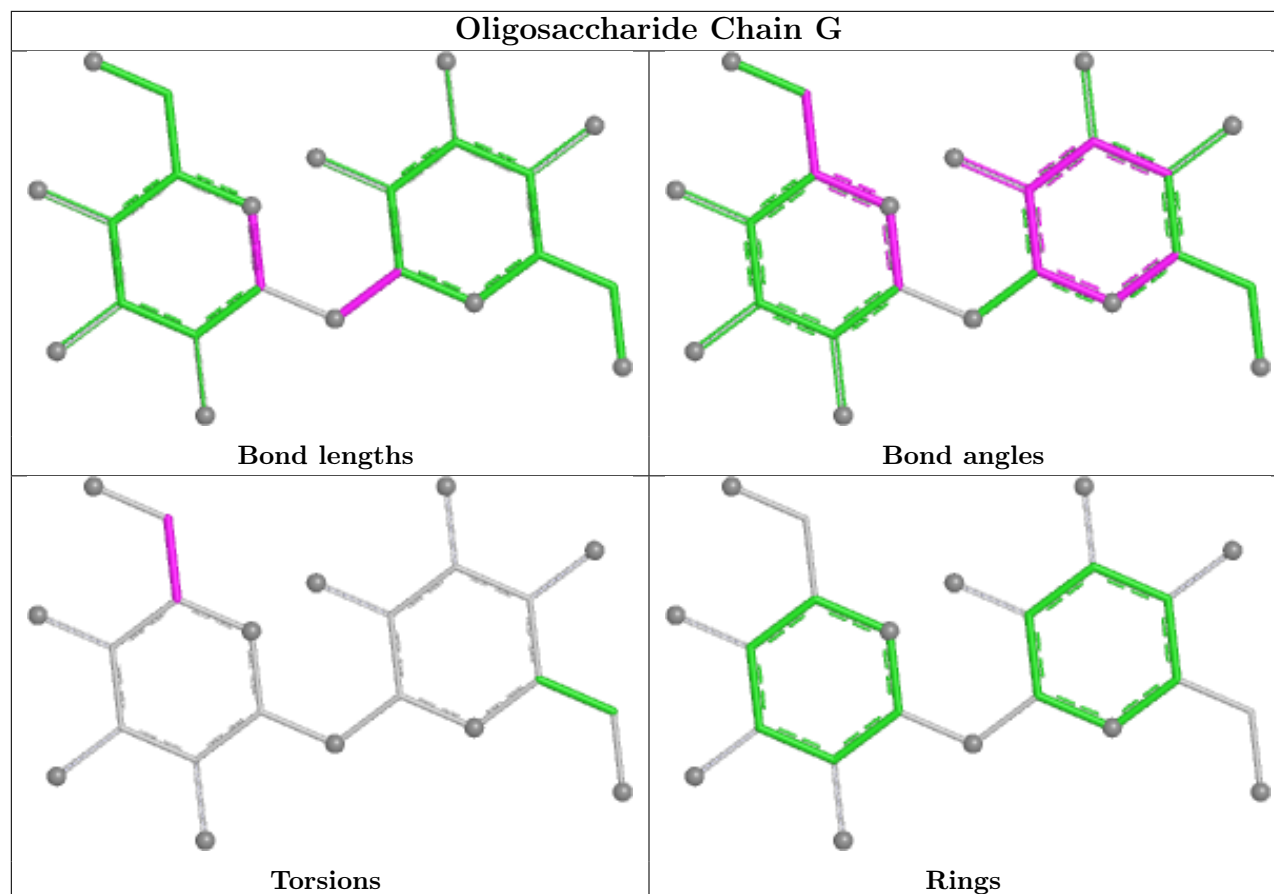
15 monomers are involved in 26 short contacts:

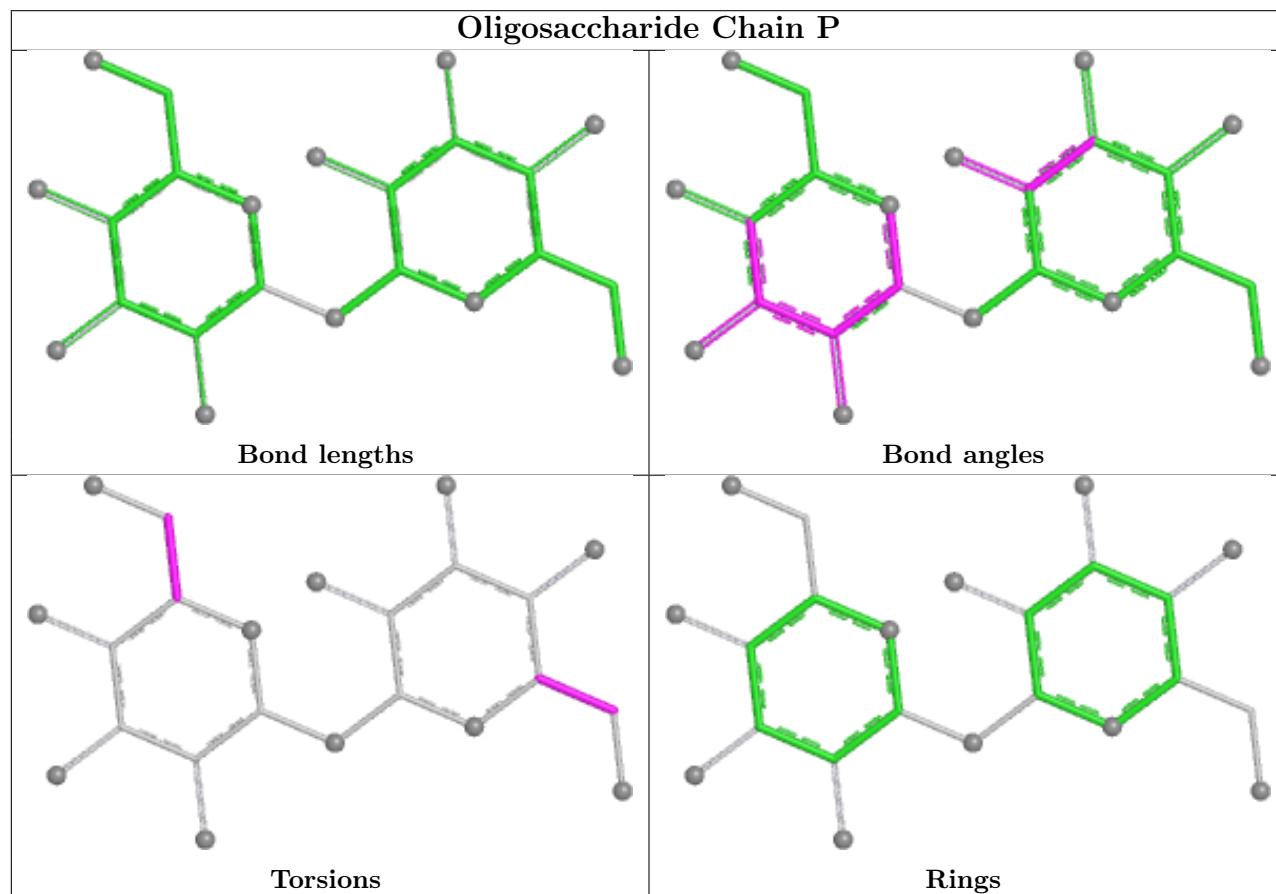
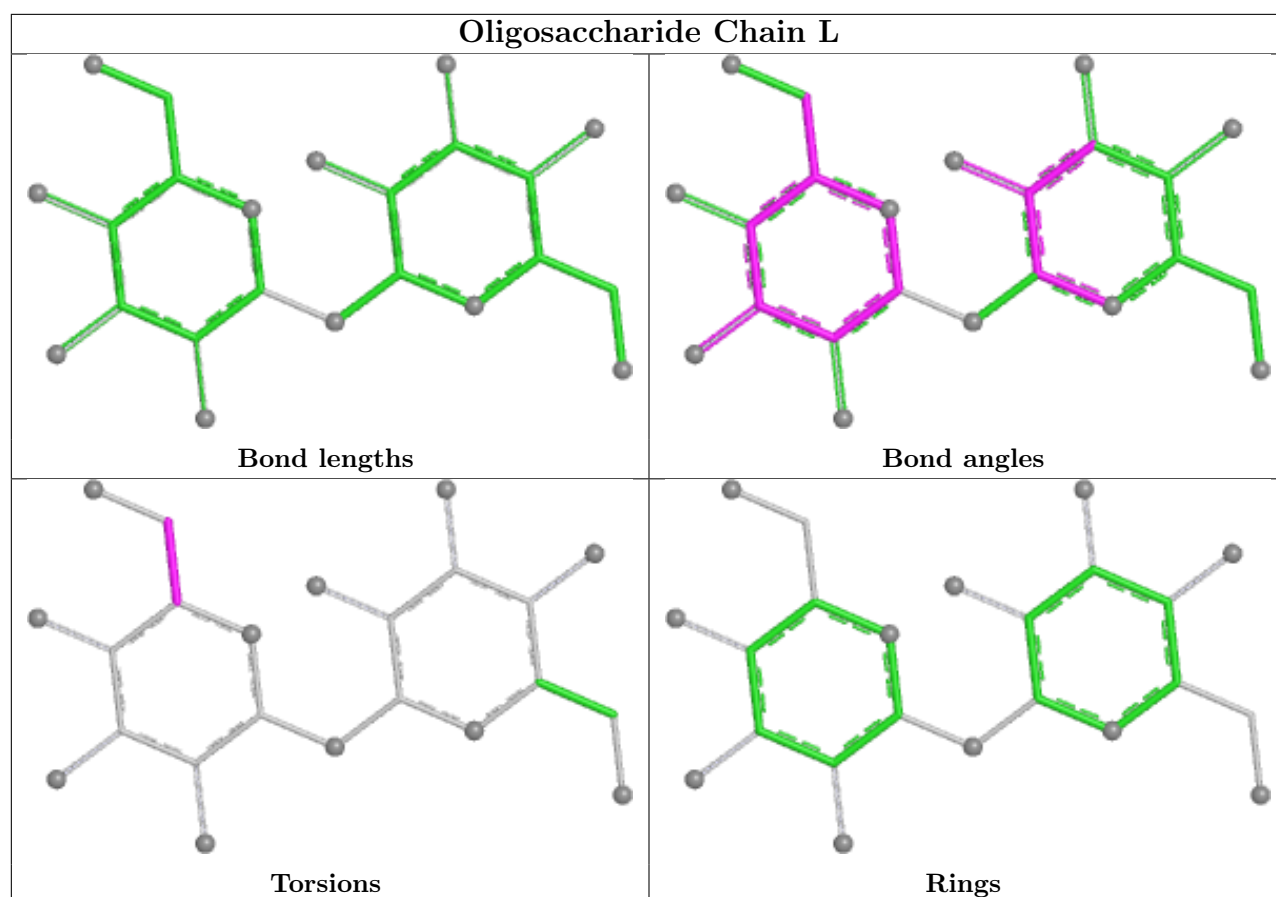


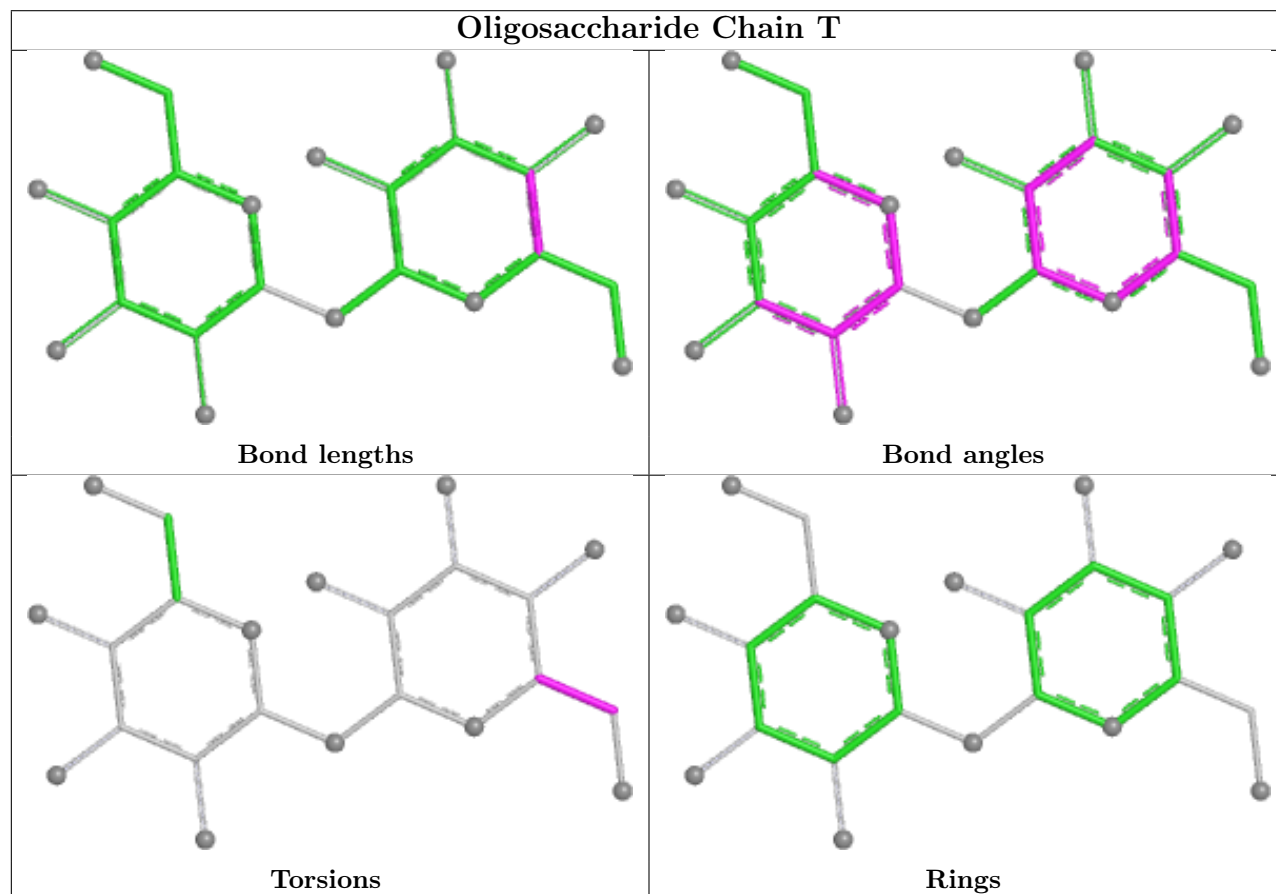
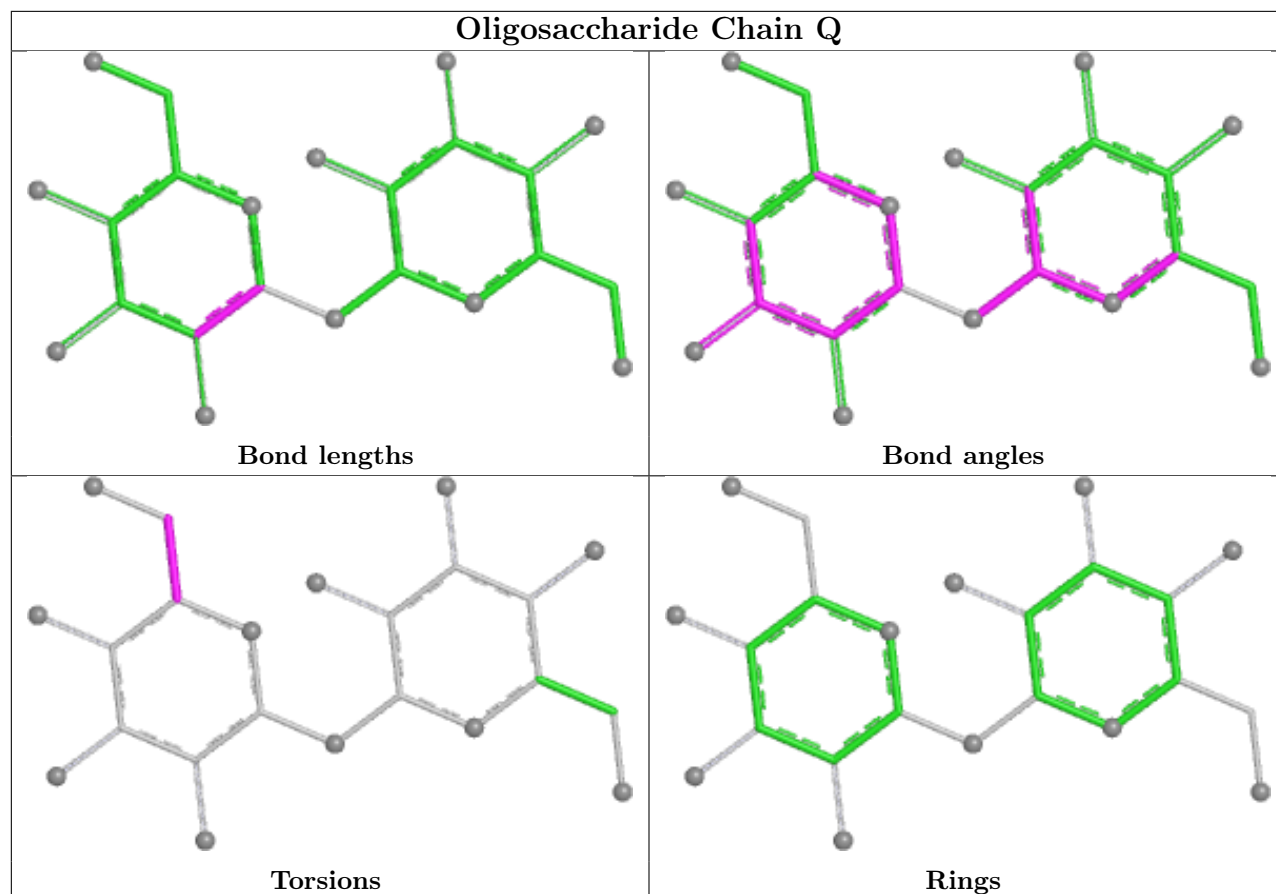
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	GLC	3	0
2	G	2	GLC	2	0
2	G	1	GLC	2	0
3	Y	1	GLC	3	0
2	U	2	GLC	3	0
3	R	1	GLC	1	0
2	P	1	GLC	1	0
2	W	1	GLC	1	0
2	W	2	GLC	6	0
3	N	2	GLC	1	0
2	E	2	GLC	1	0
2	E	1	GLC	1	0
3	S	1	GLC	2	0
2	U	1	GLC	4	0
2	Q	2	GLC	1	0

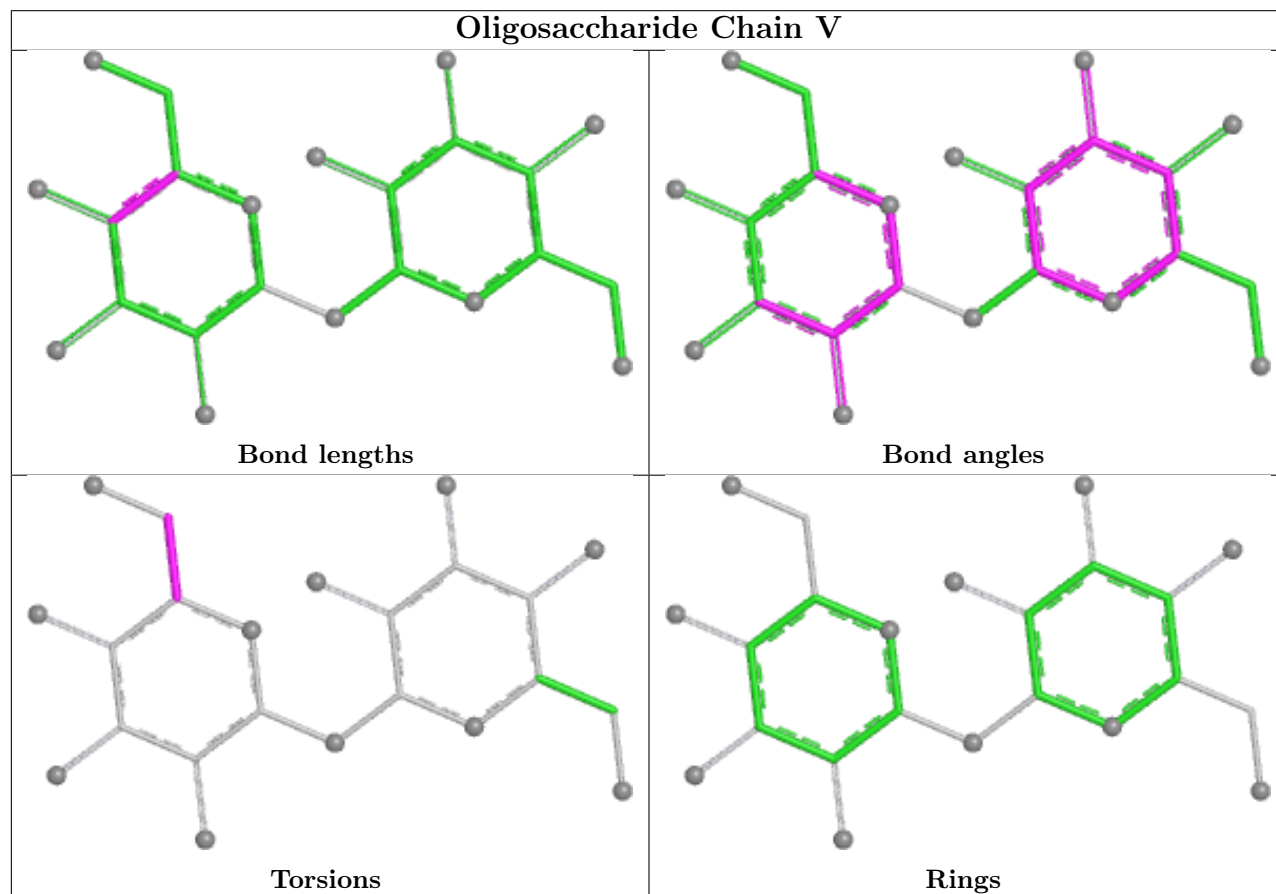
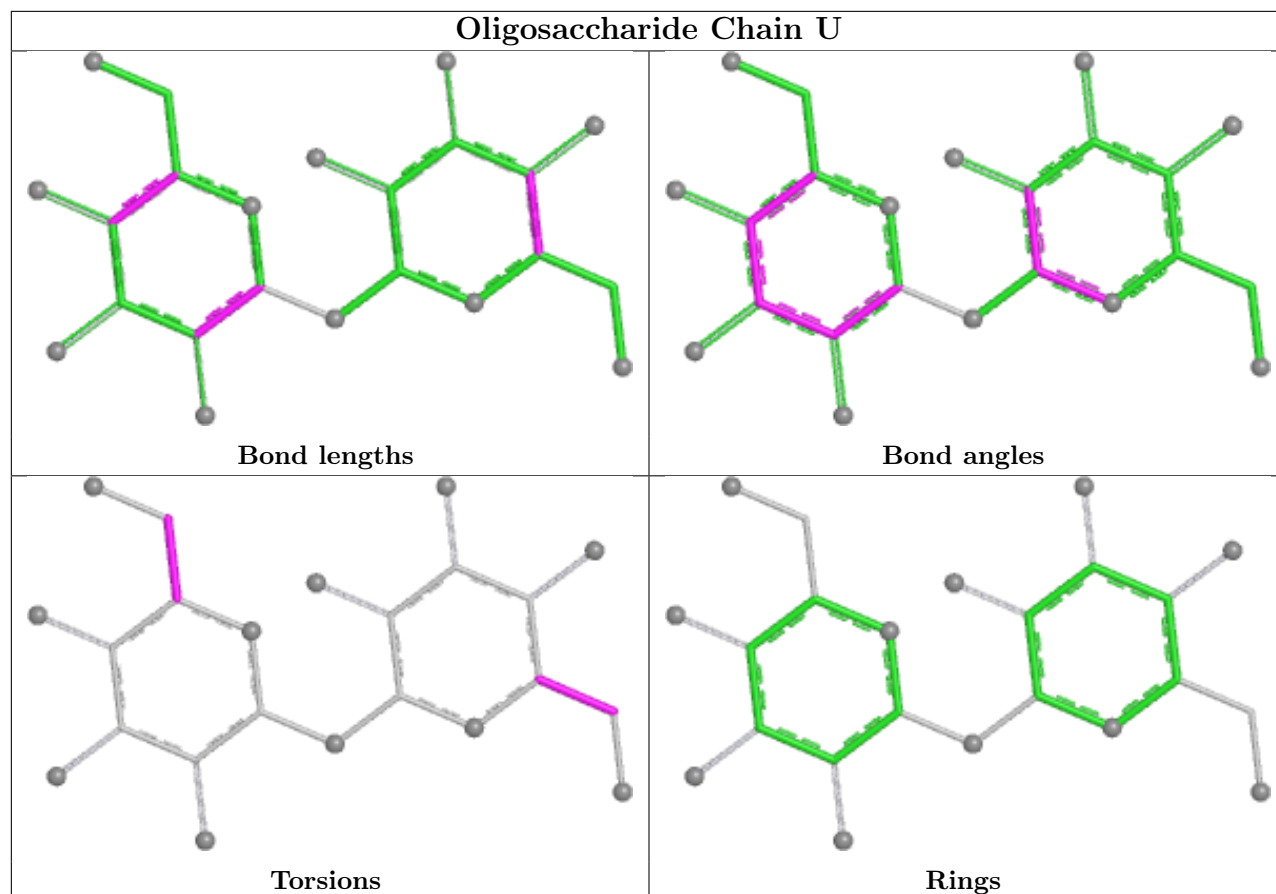
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

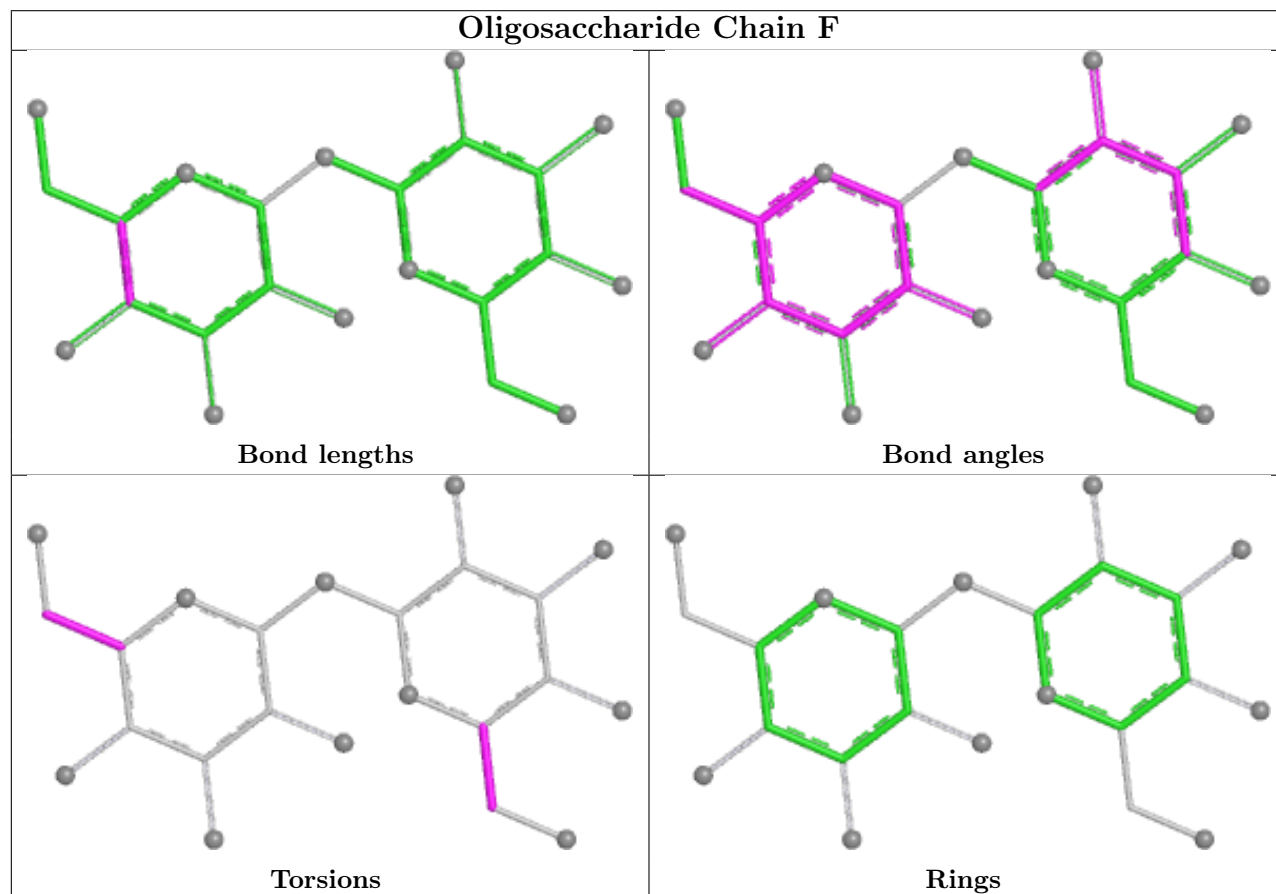
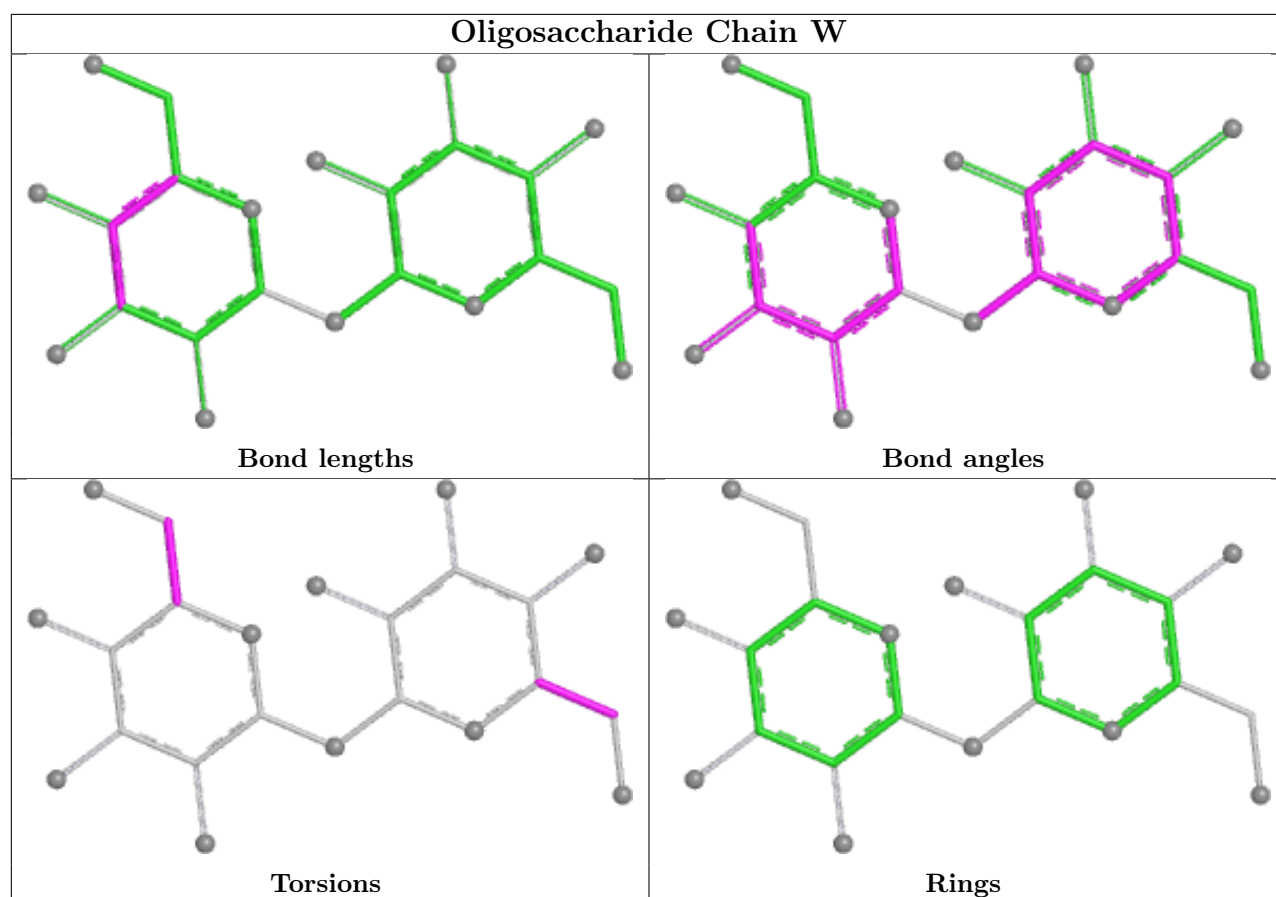


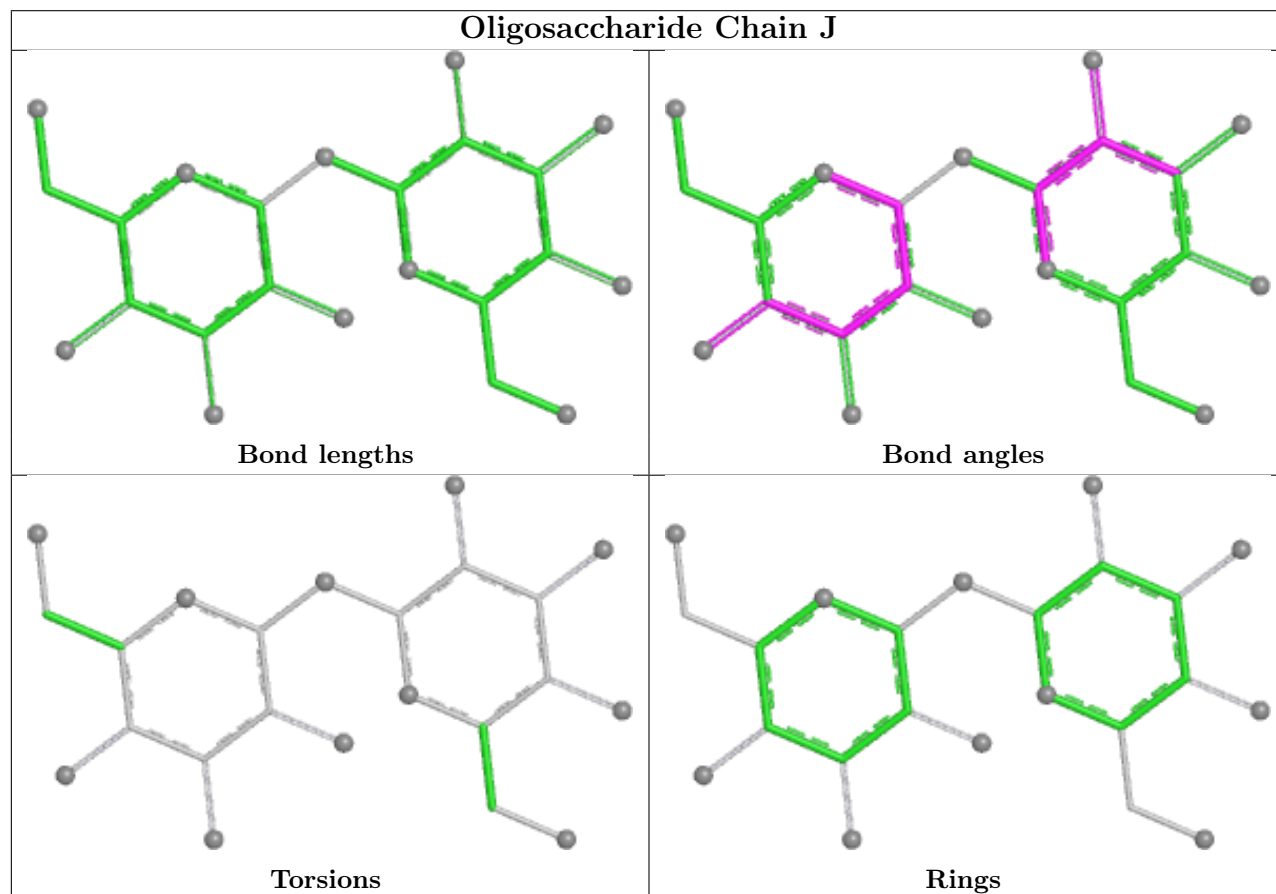
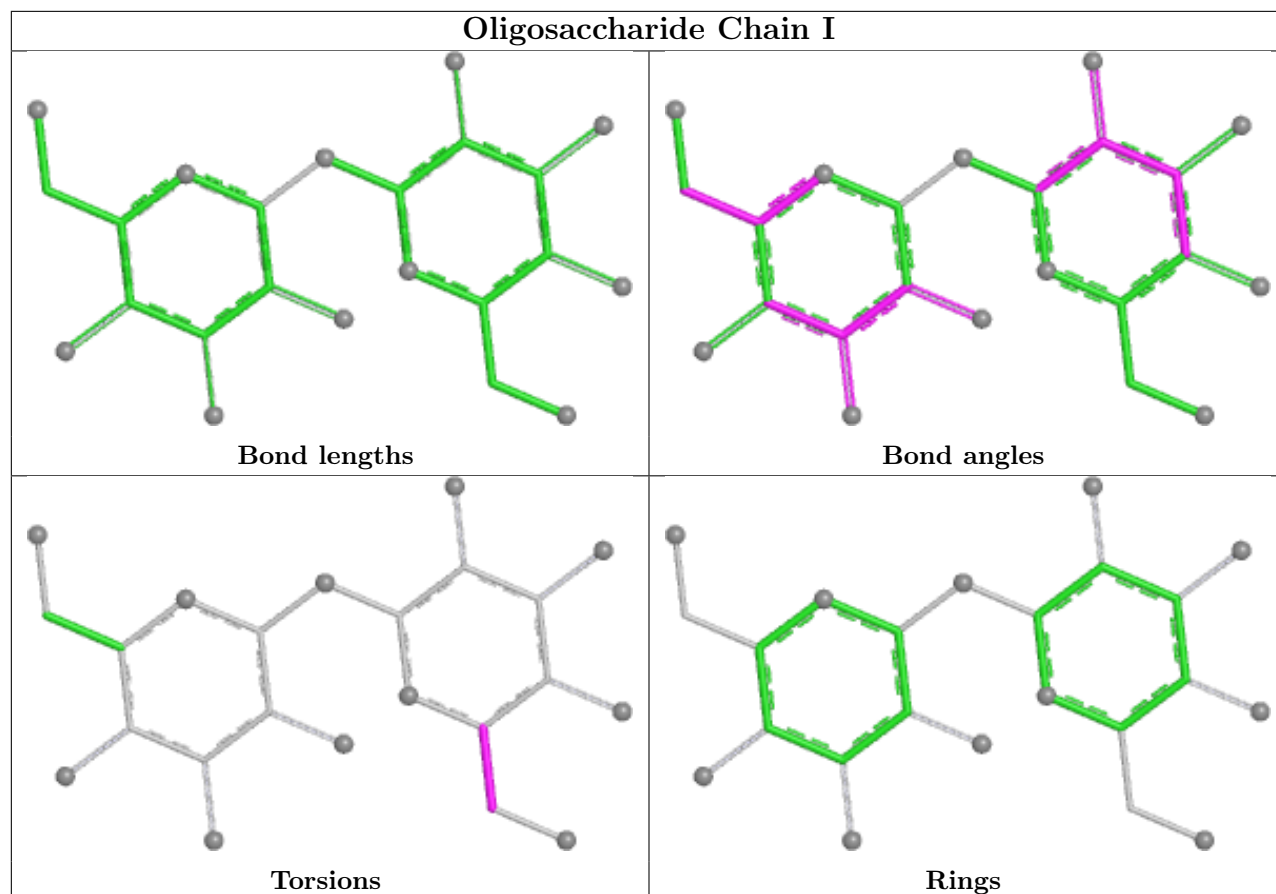


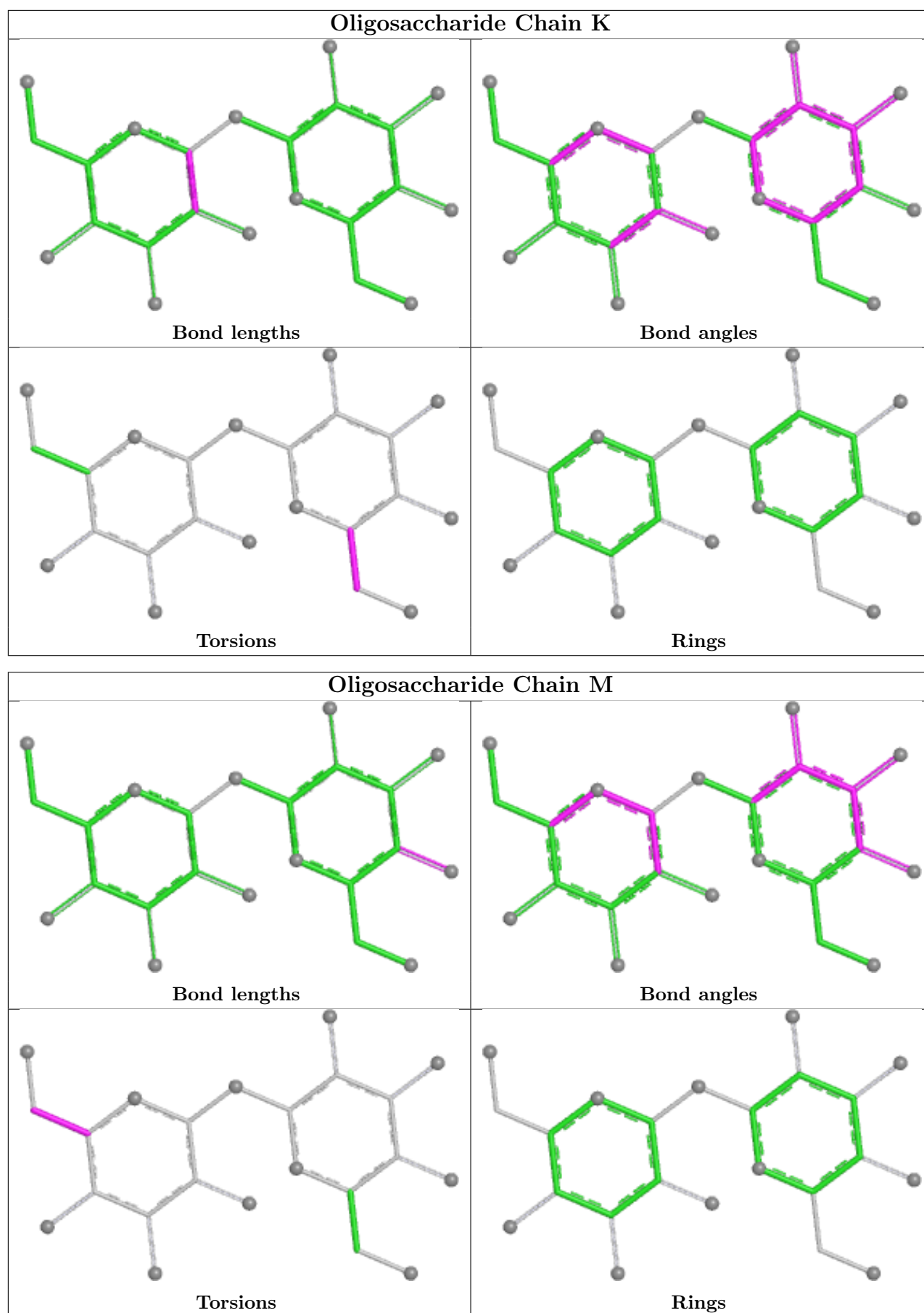




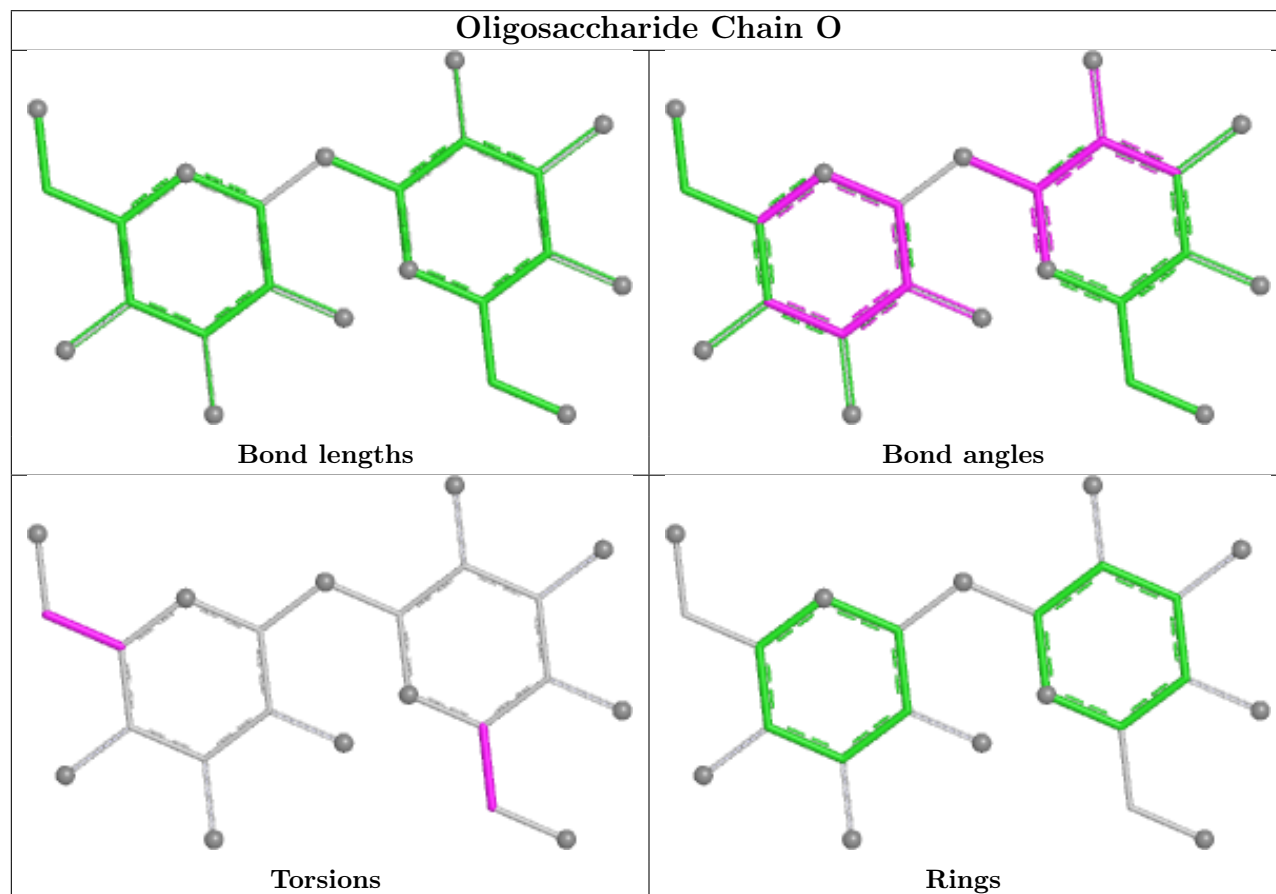
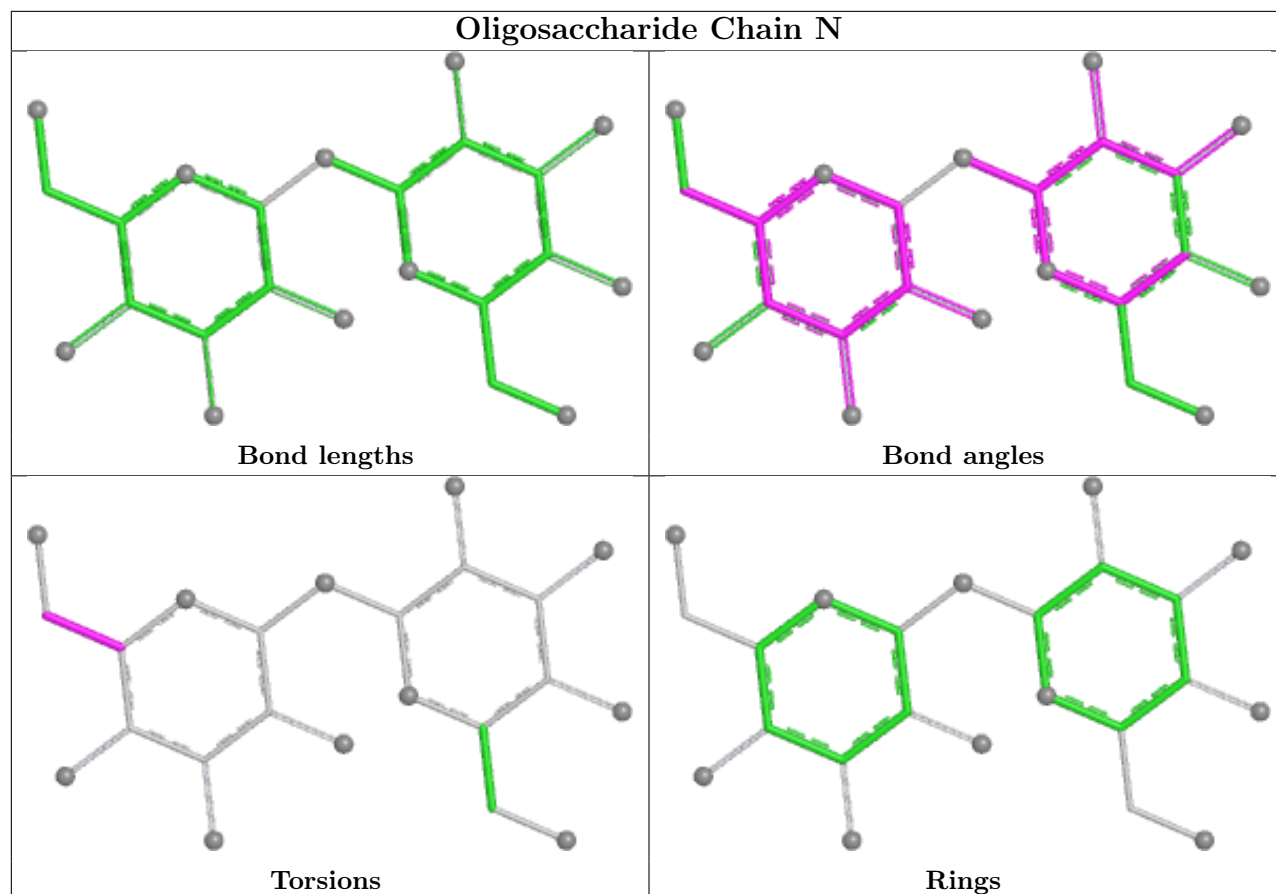


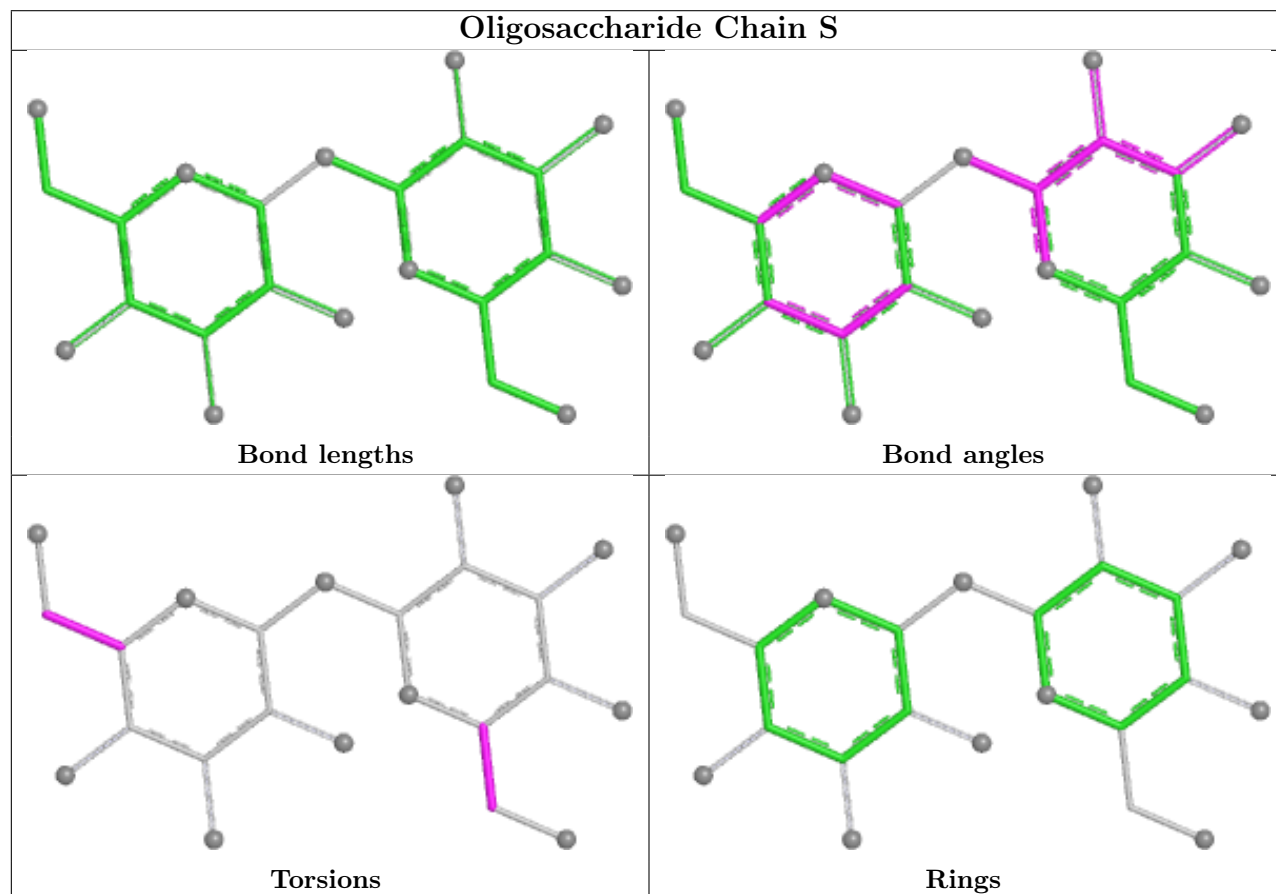
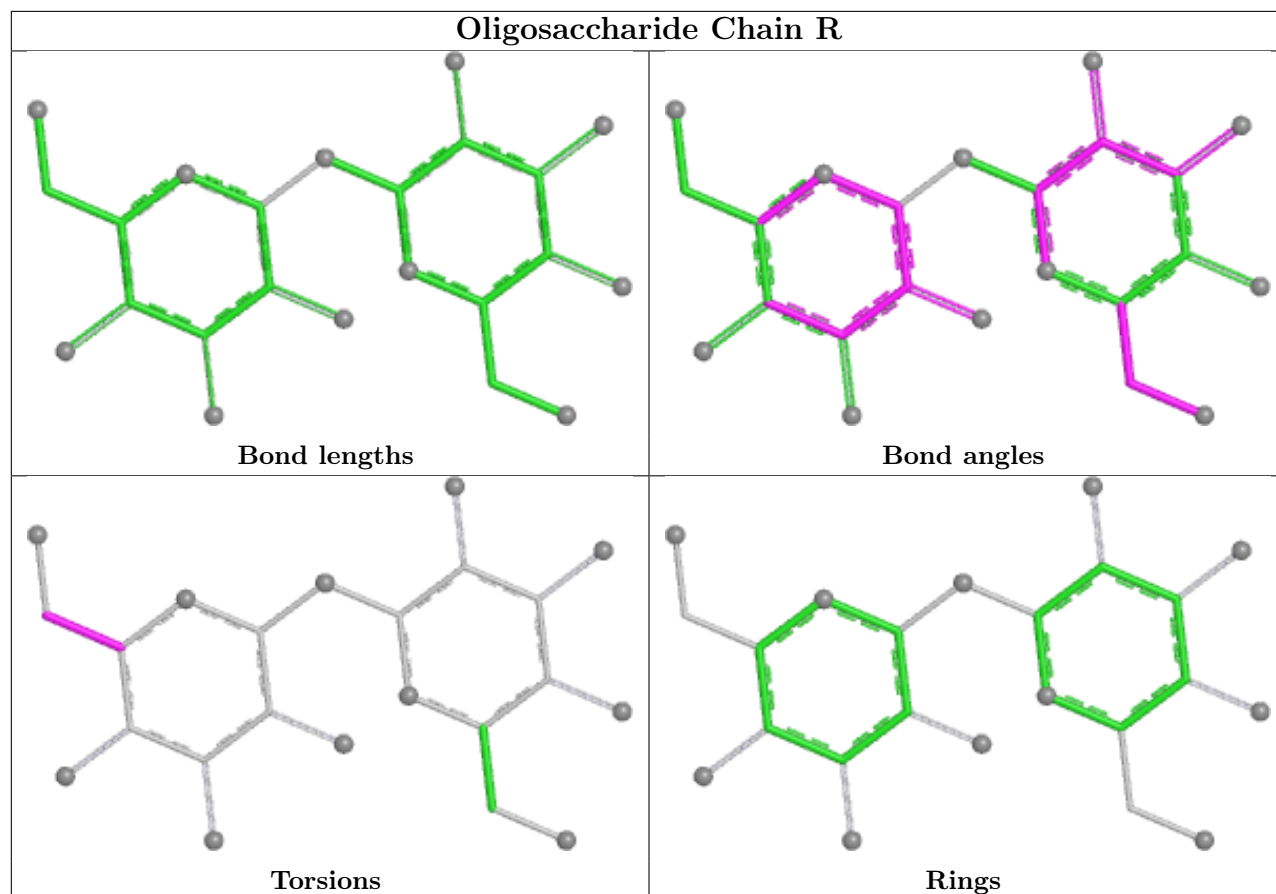


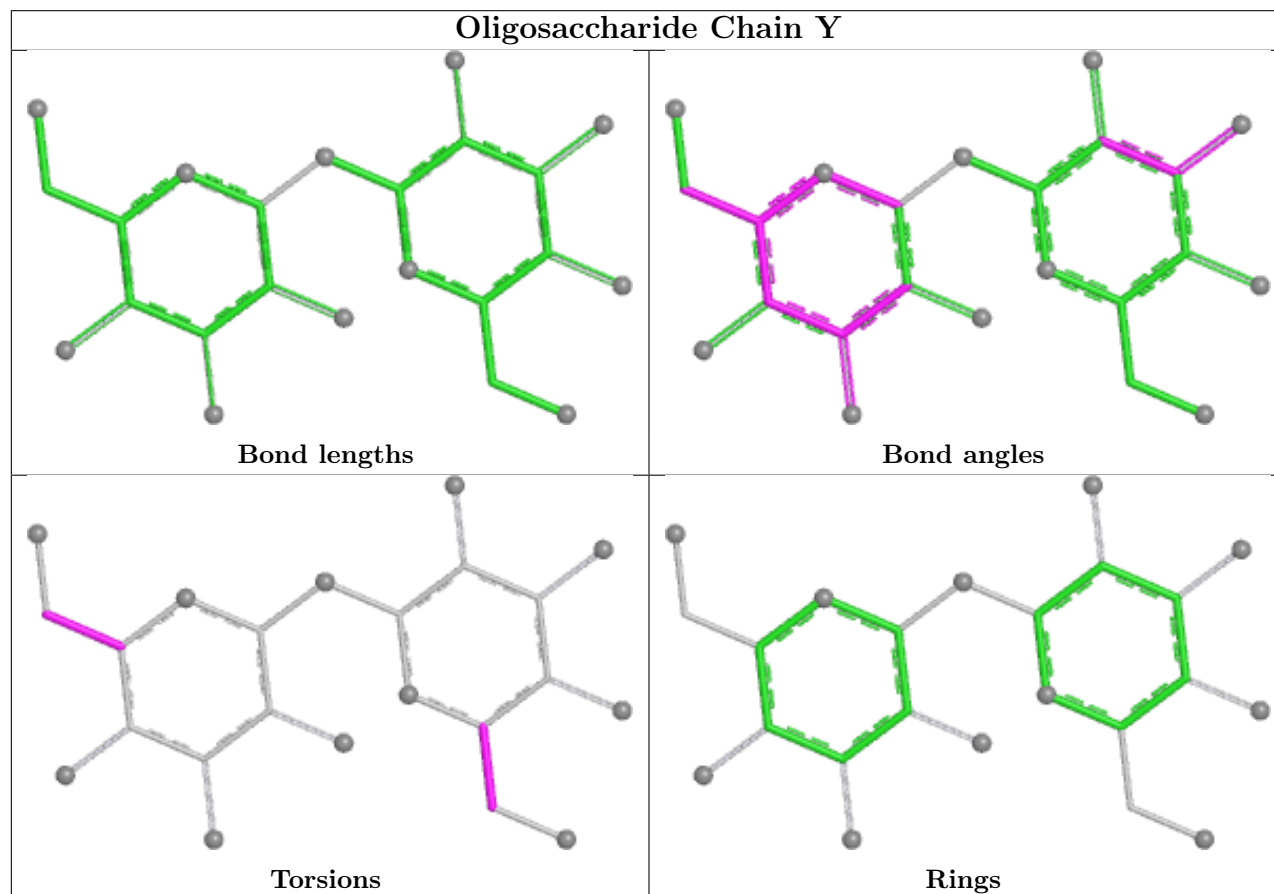
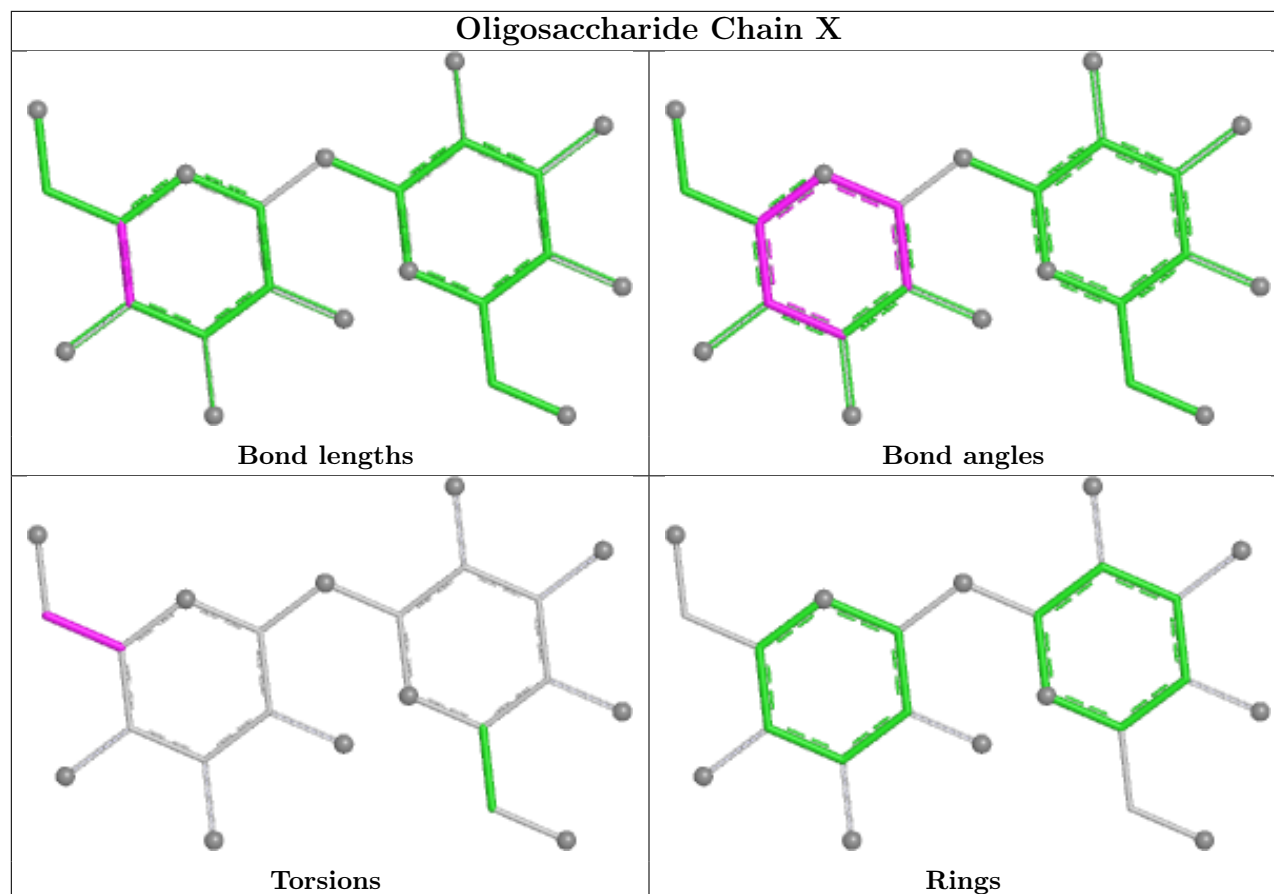


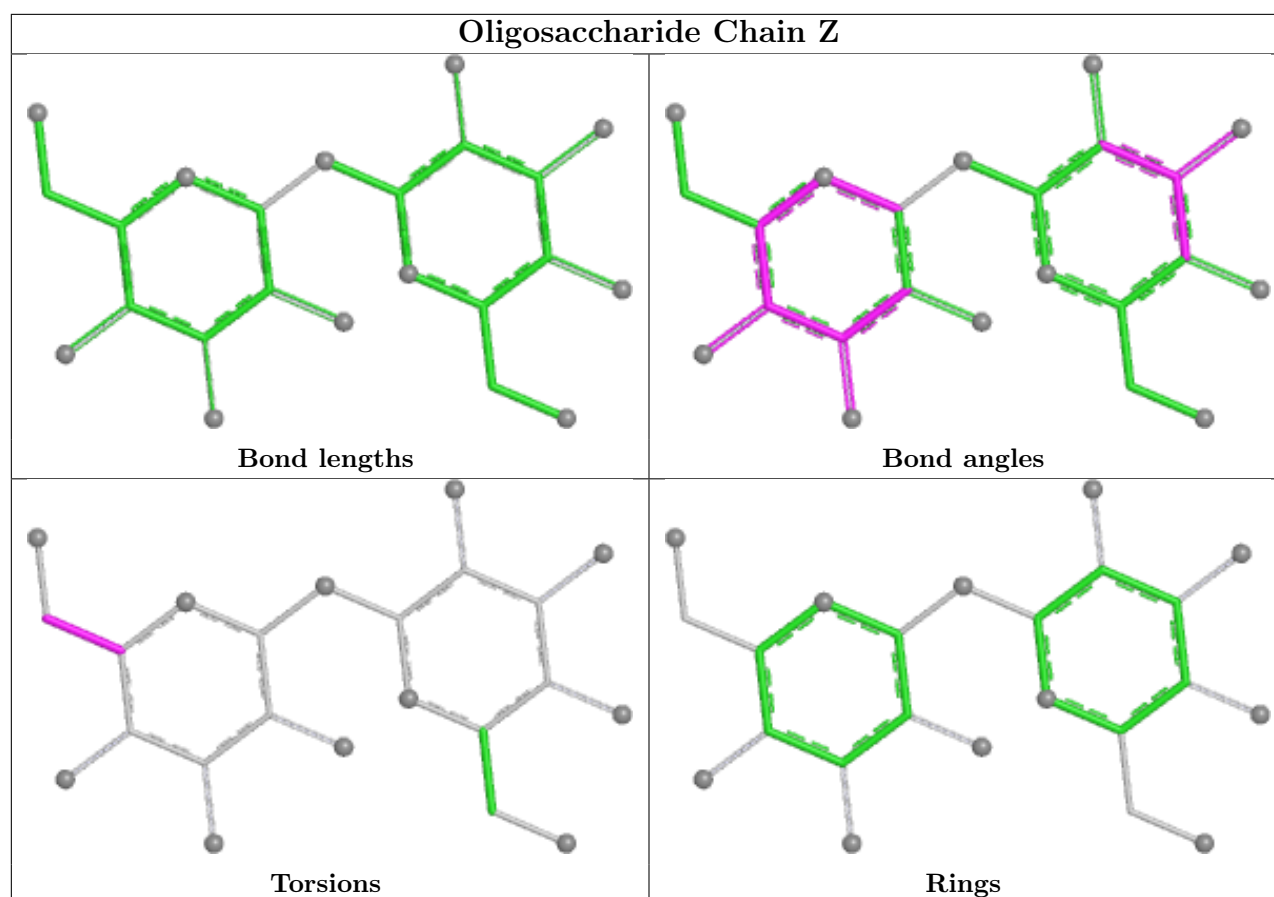












## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAD	D	501	-	42,48,48	0.87	3 (7%)	50,73,73	1.22	6 (12%)
4	NAD	C	501	-	42,48,48	1.18	3 (7%)	50,73,73	1.27	5 (10%)
4	NAD	B	501	-	42,48,48	1.08	2 (4%)	50,73,73	1.25	6 (12%)
4	NAD	A	501	-	42,48,48	0.95	1 (2%)	50,73,73	1.14	6 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	D	501	-	-	6/26/62/62	0/5/5/5
4	NAD	C	501	-	-	7/26/62/62	0/5/5/5
4	NAD	B	501	-	-	4/26/62/62	0/5/5/5
4	NAD	A	501	-	-	5/26/62/62	0/5/5/5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	NAD	PA-O3	4.23	1.64	1.59
4	B	501	NAD	C2N-N1N	3.95	1.39	1.35
4	A	501	NAD	C2N-N1N	3.70	1.39	1.35
4	B	501	NAD	O4D-C1D	3.46	1.45	1.40
4	C	501	NAD	O4D-C1D	3.24	1.45	1.40

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	NAD	C2N-C3N-C4N	3.53	122.36	118.26
4	C	501	NAD	C6N-N1N-C2N	-3.39	119.00	121.88
4	B	501	NAD	C2N-C3N-C4N	3.08	121.84	118.26
4	D	501	NAD	C6N-N1N-C2N	-3.07	119.27	121.88
4	C	501	NAD	C4N-C3N-C7N	-2.95	113.02	121.06

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	NAD	O4D-C1D-N1N-C2N
4	A	501	NAD	O4D-C1D-N1N-C6N
4	A	501	NAD	C2D-C1D-N1N-C2N
4	A	501	NAD	C2D-C1D-N1N-C6N
4	B	501	NAD	O4D-C1D-N1N-C6N

There are no ring outliers.

4 monomers are involved in 10 short contacts:

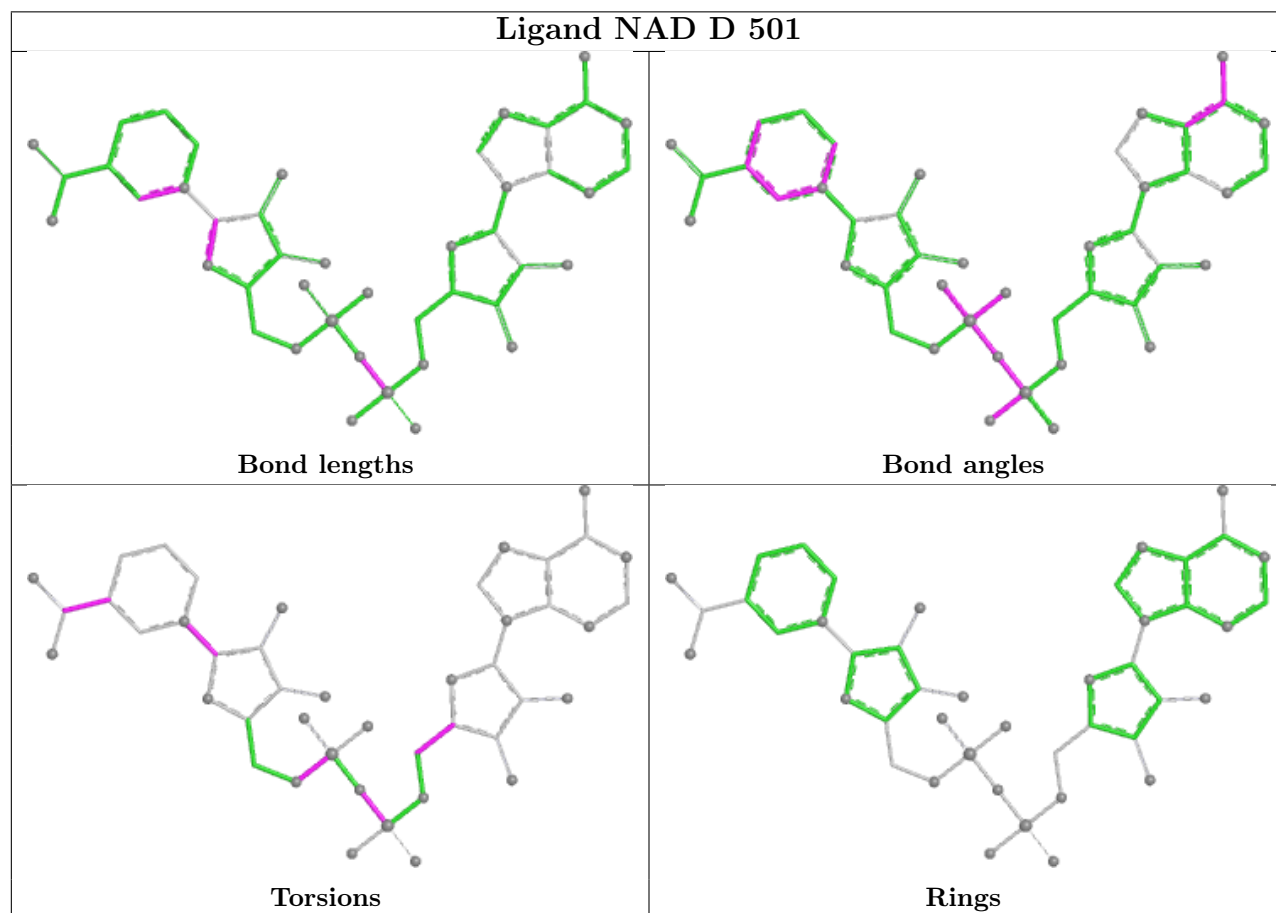
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	501	NAD	2	0

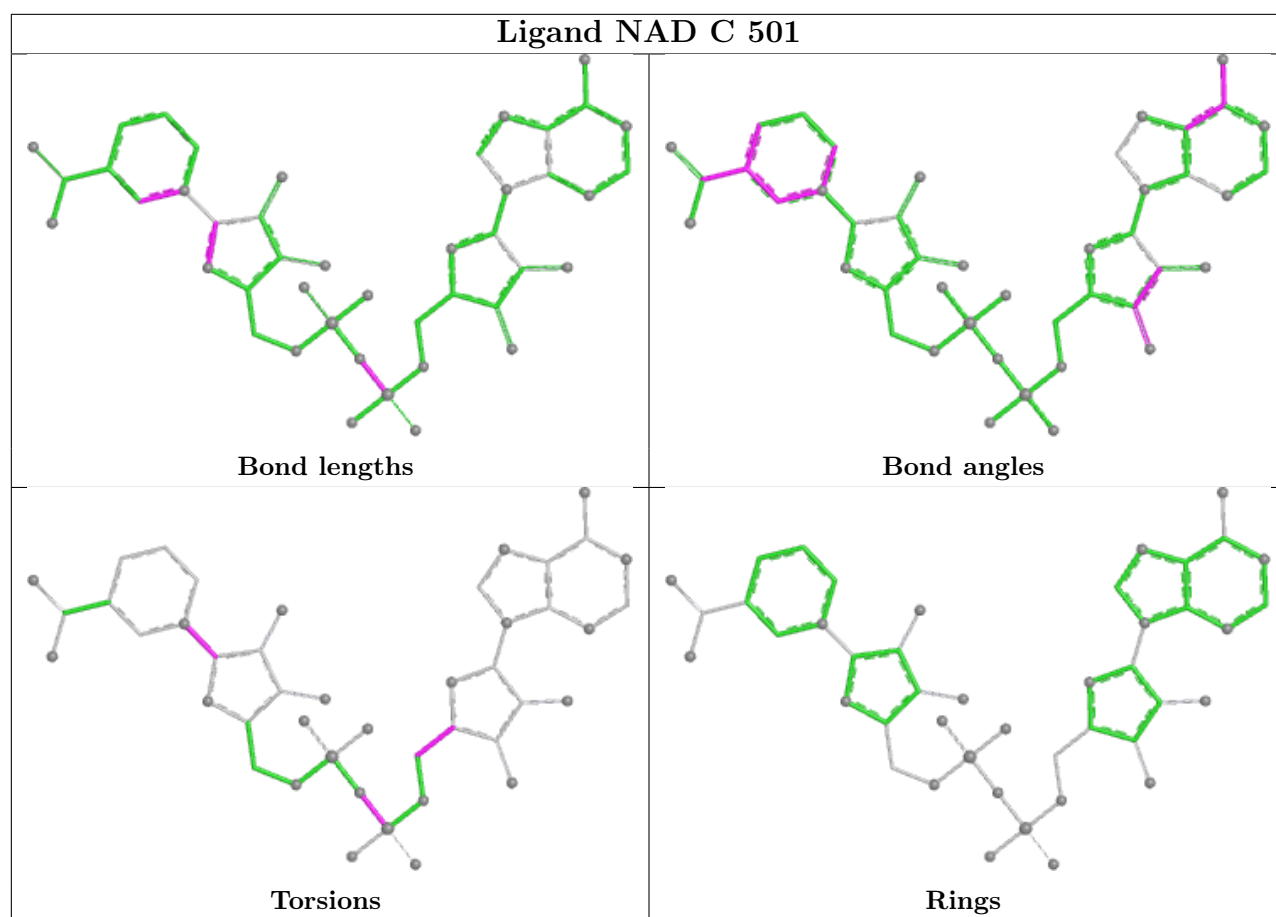
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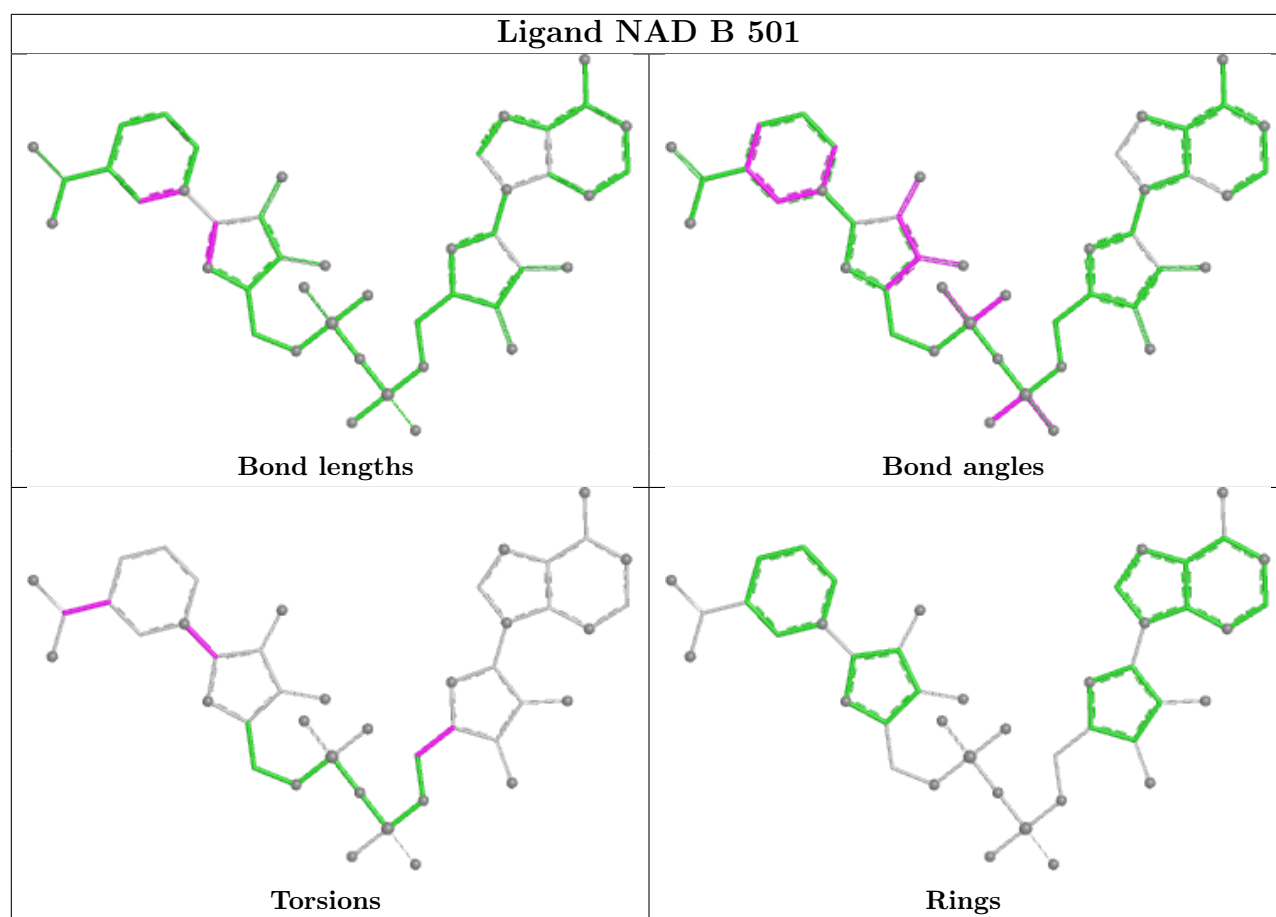
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	NAD	2	0
4	B	501	NAD	3	0
4	A	501	NAD	3	0

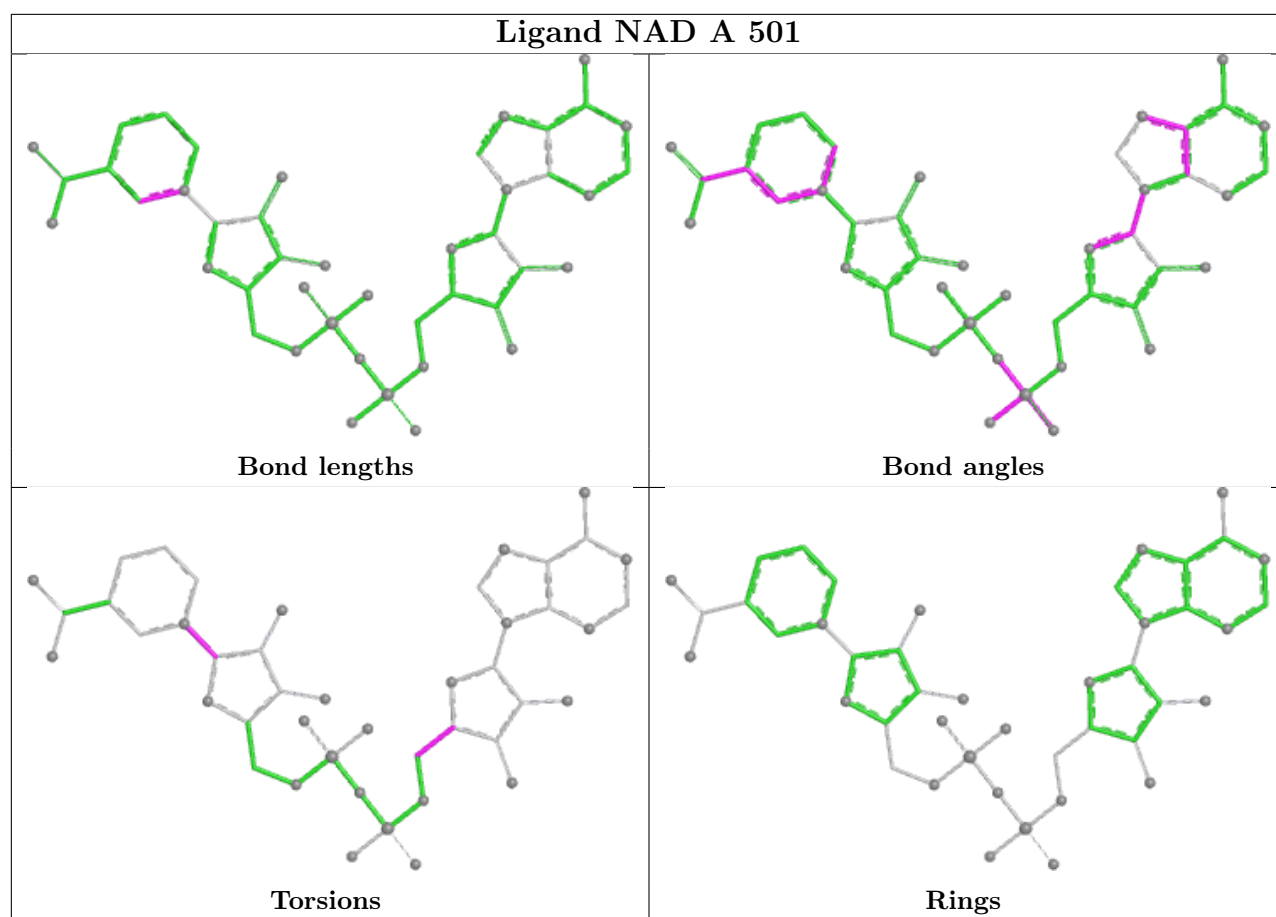
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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](#)

EDS failed to run properly - this section is therefore empty.

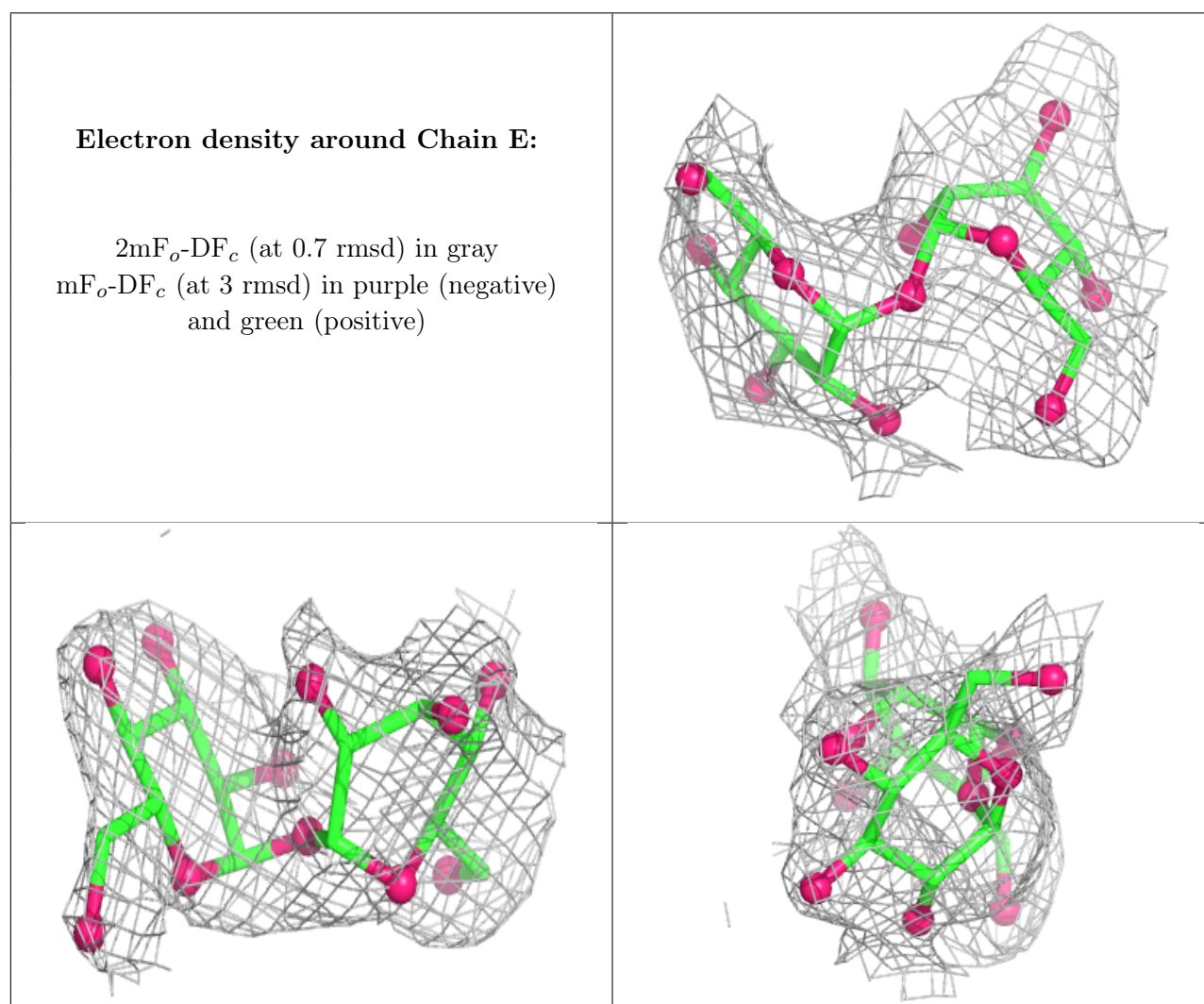
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

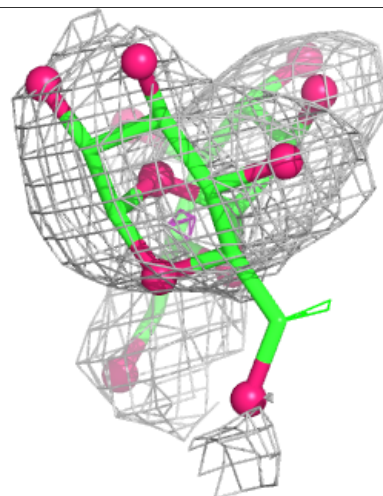
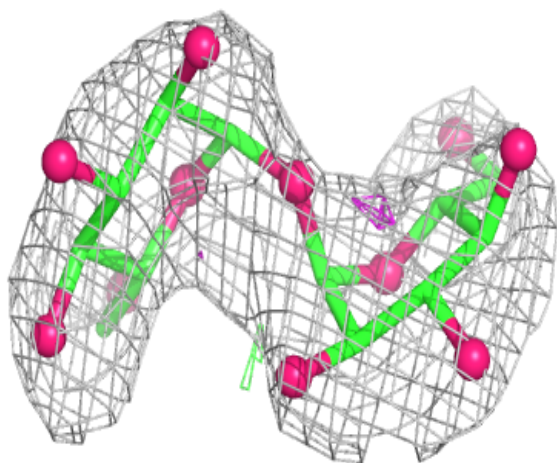
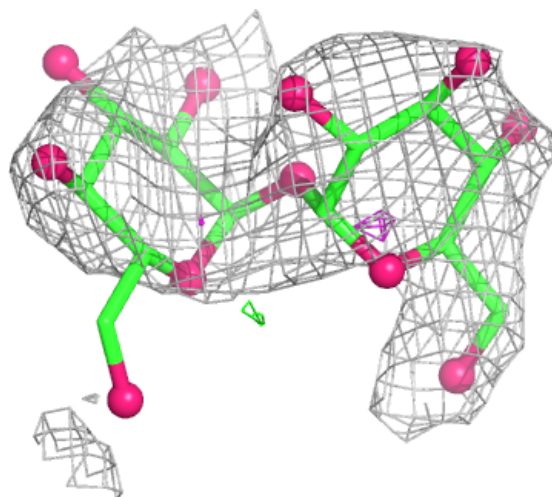
EDS failed to run properly - this section is therefore empty.

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.



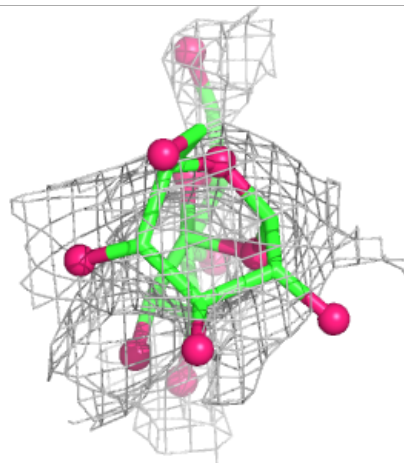
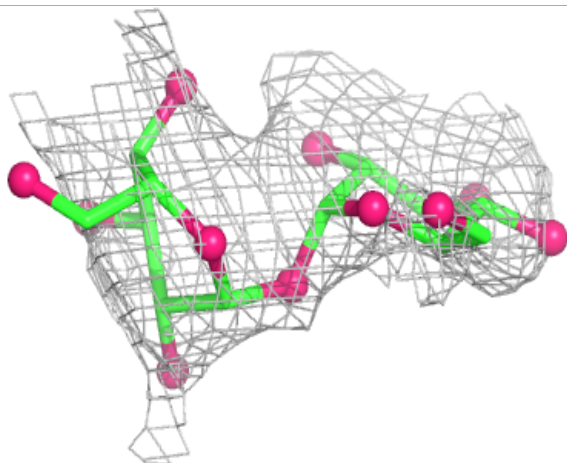
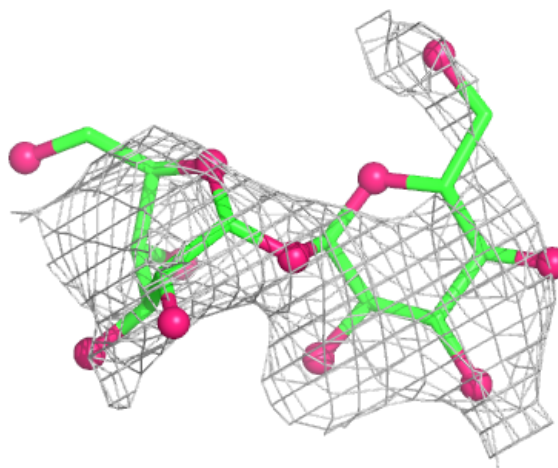
**Electron density around Chain G:**

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



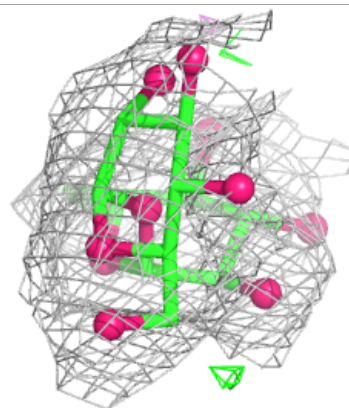
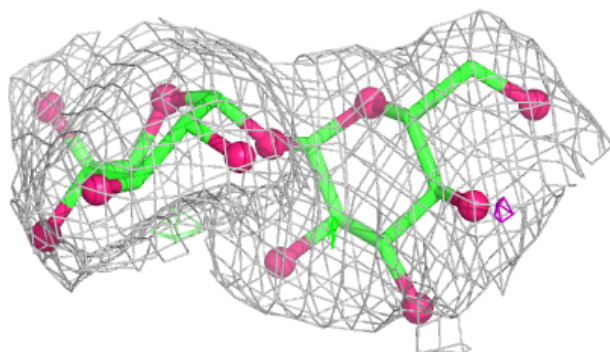
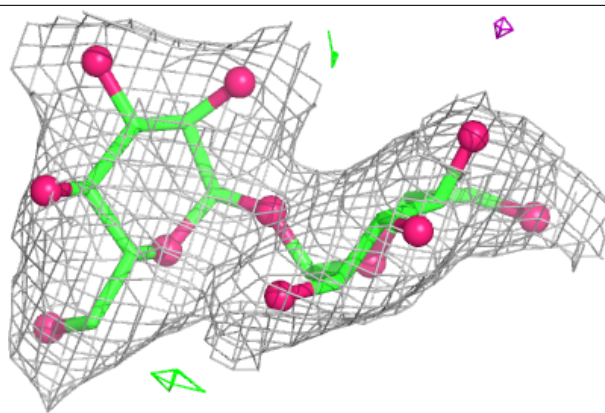
**Electron density around Chain H:**

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



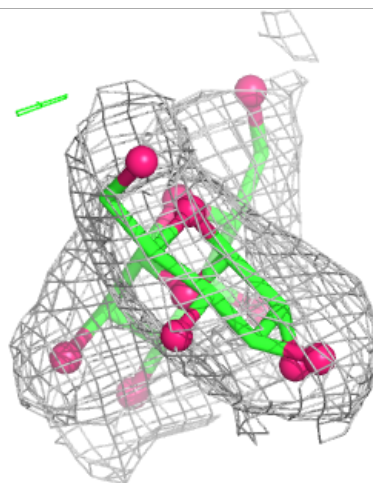
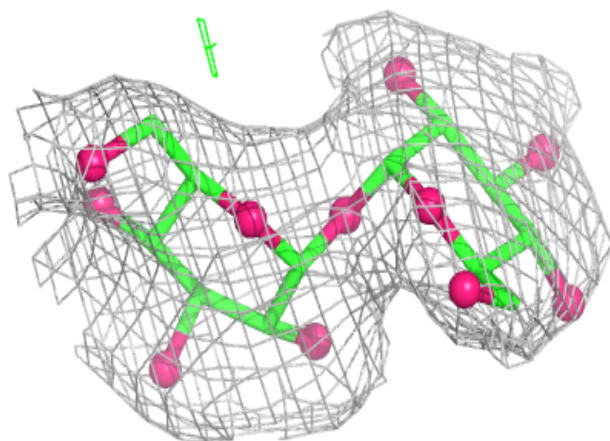
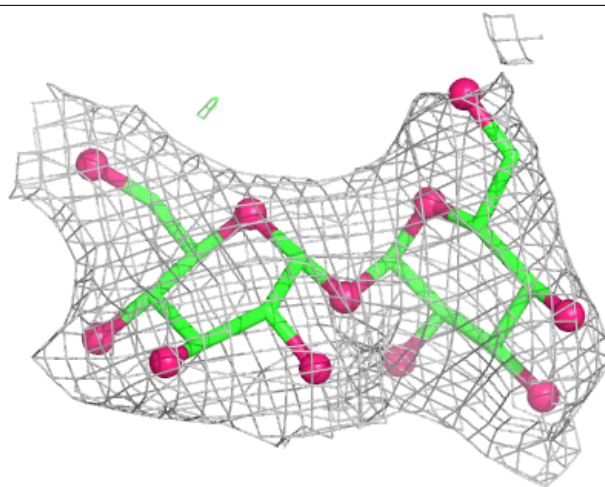
**Electron density around Chain L:**

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



**Electron density around Chain P:**

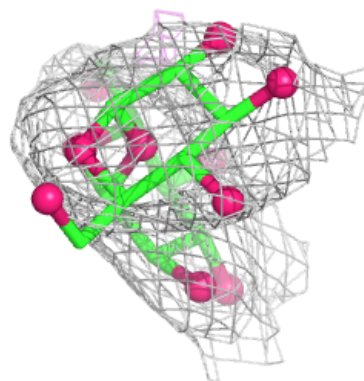
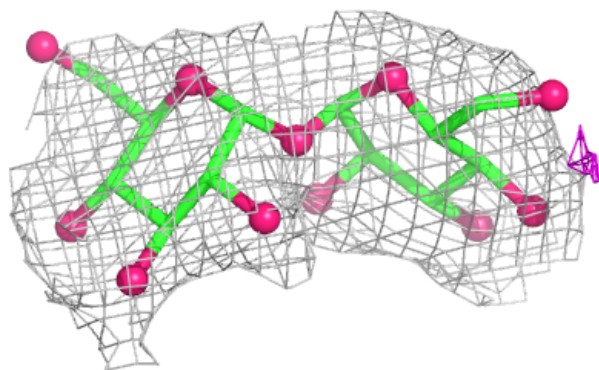
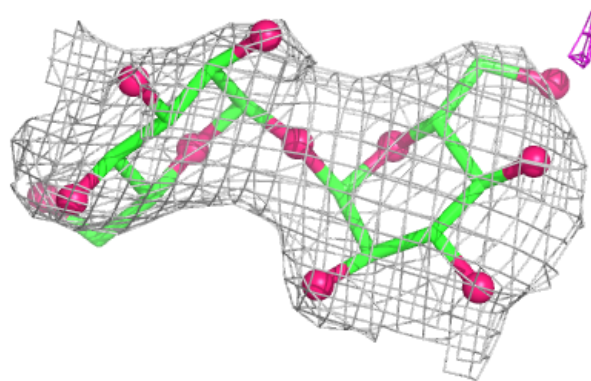
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





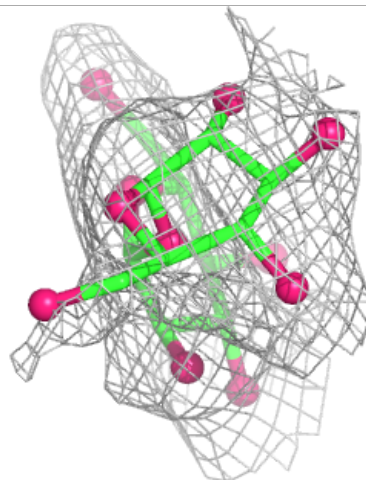
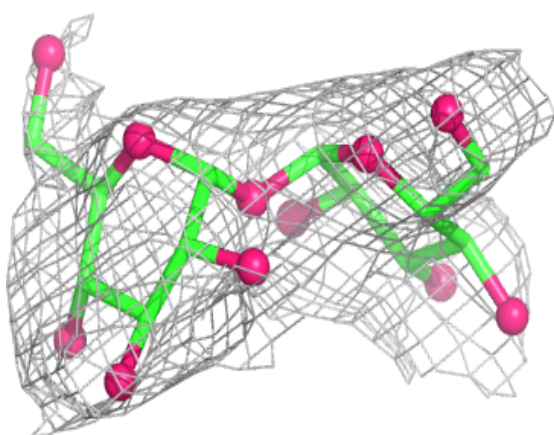
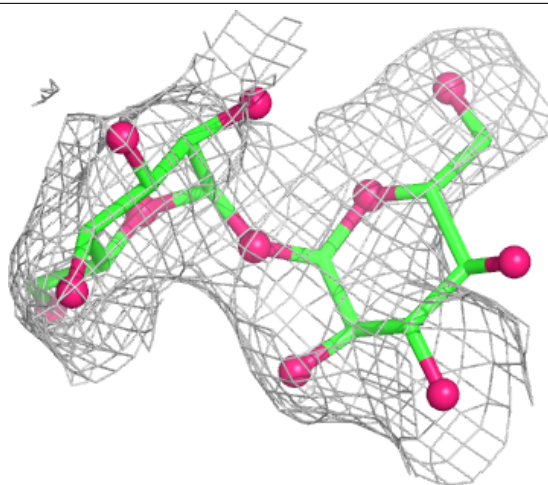
**Electron density around Chain Q:**

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



**Electron density around Chain T:**

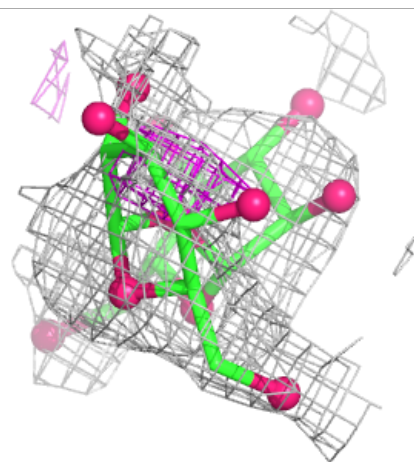
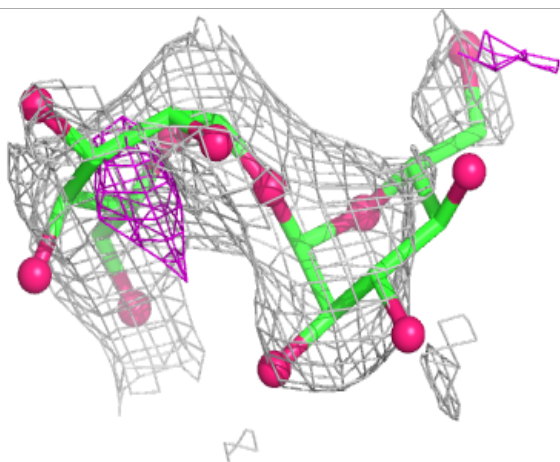
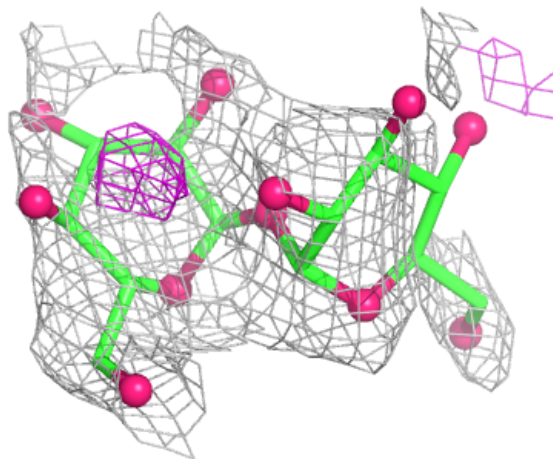
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





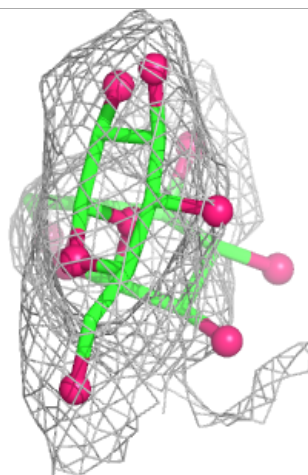
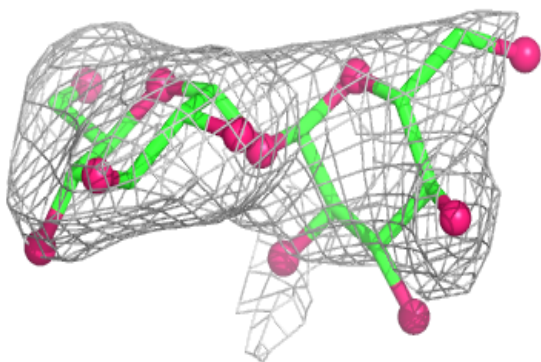
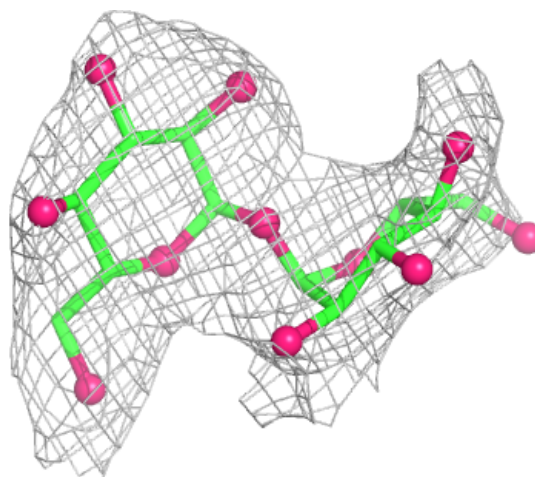
**Electron density around Chain U:**

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



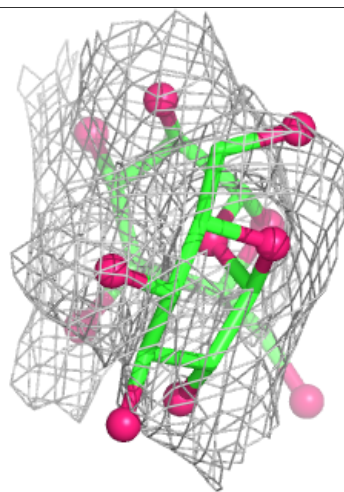
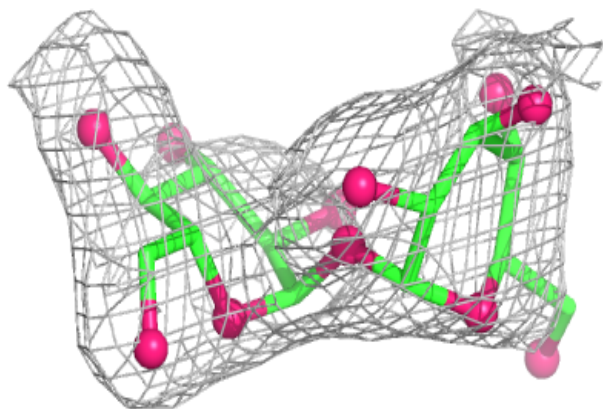
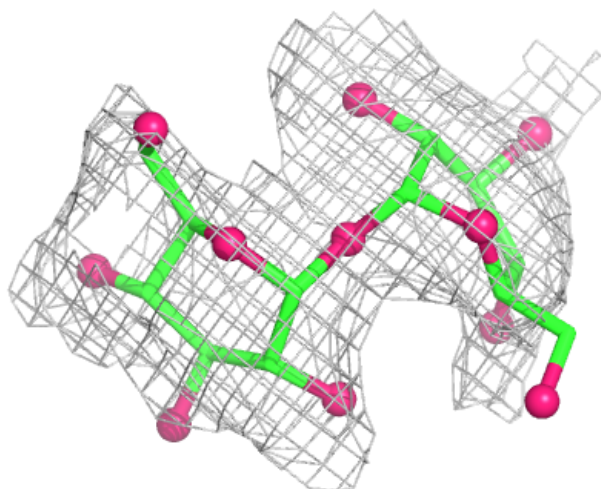
**Electron density around Chain V:**

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



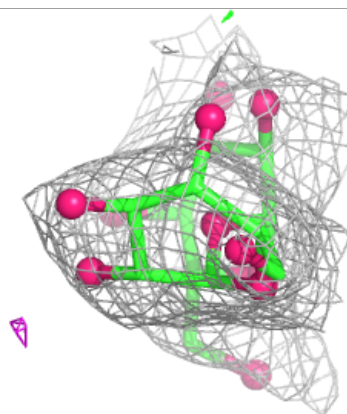
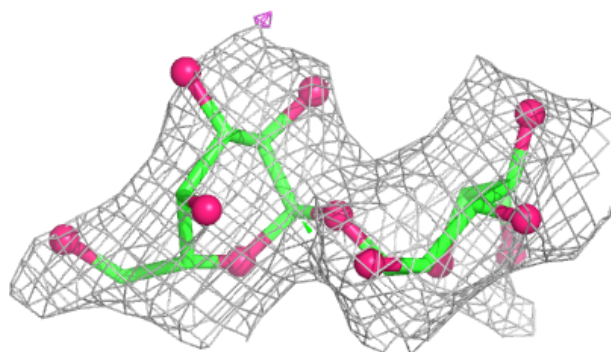
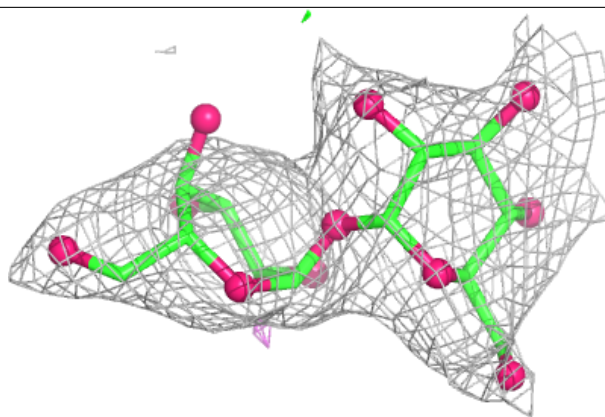
**Electron density around Chain W:**

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

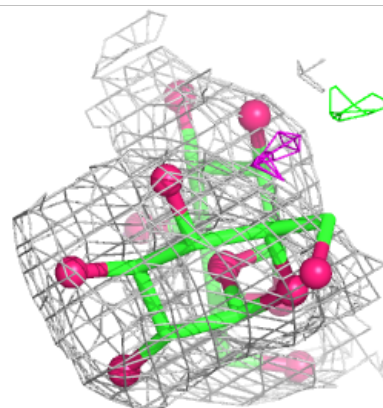
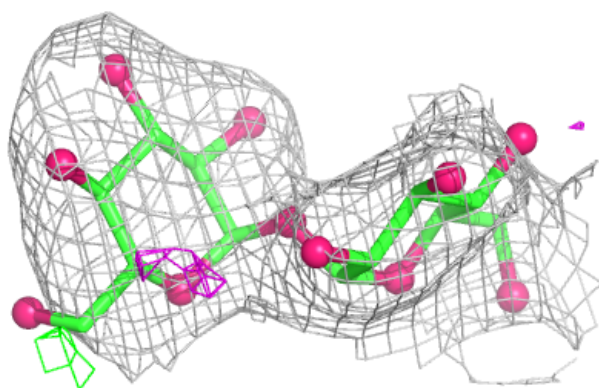
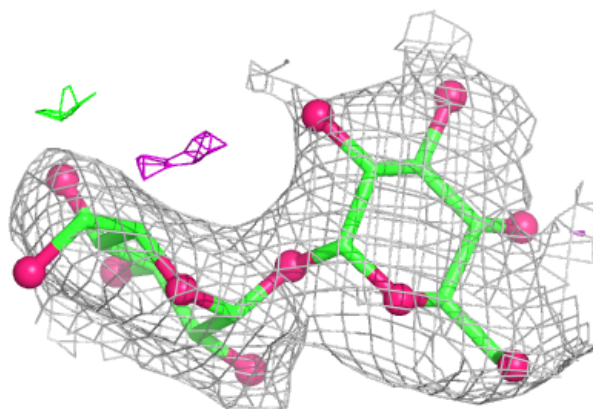


**Electron density around Chain F:**

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

**Electron density around Chain I:**

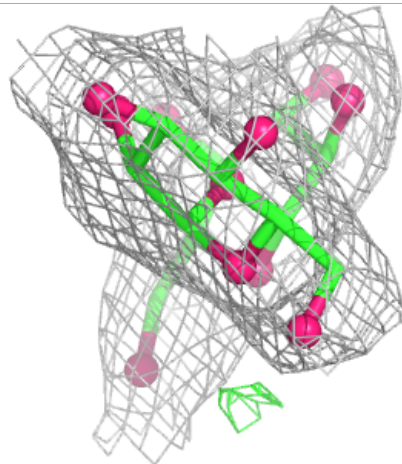
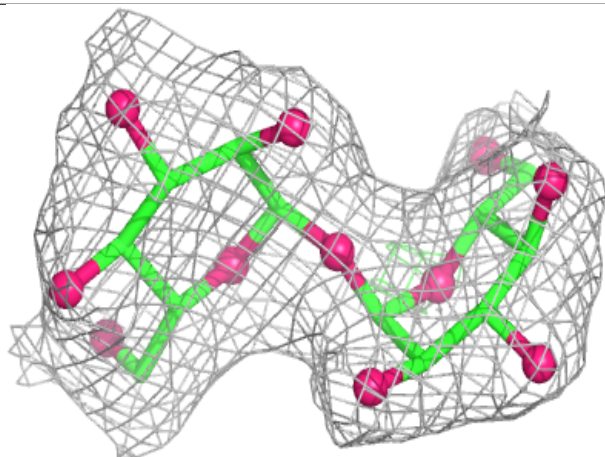
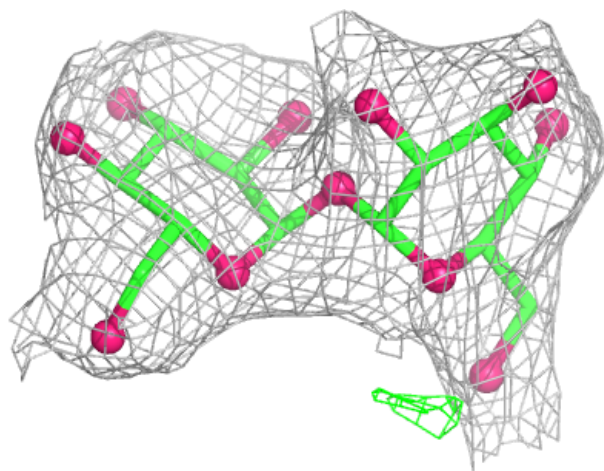
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





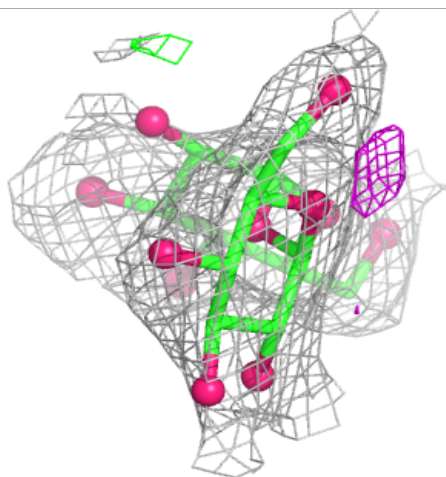
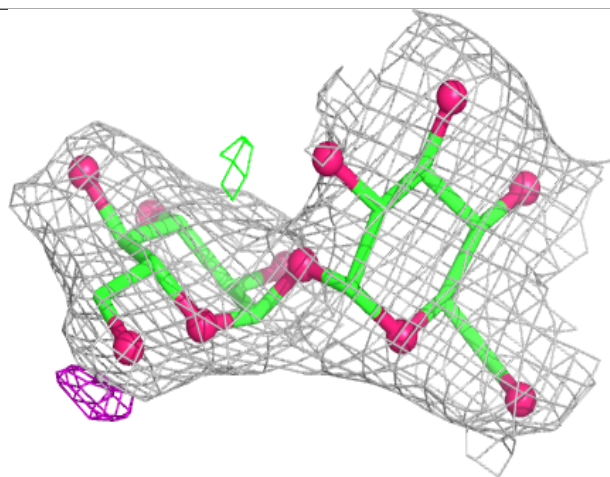
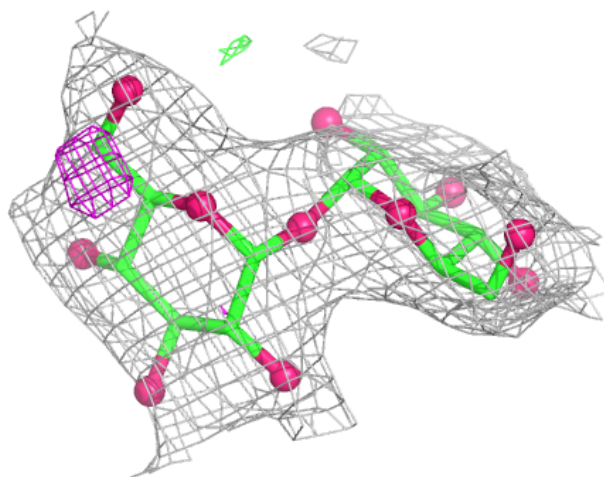
**Electron density around Chain J:**

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



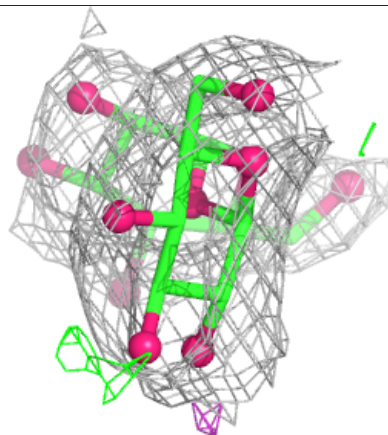
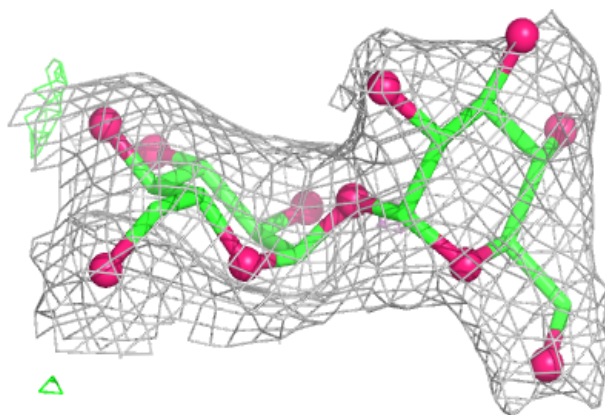
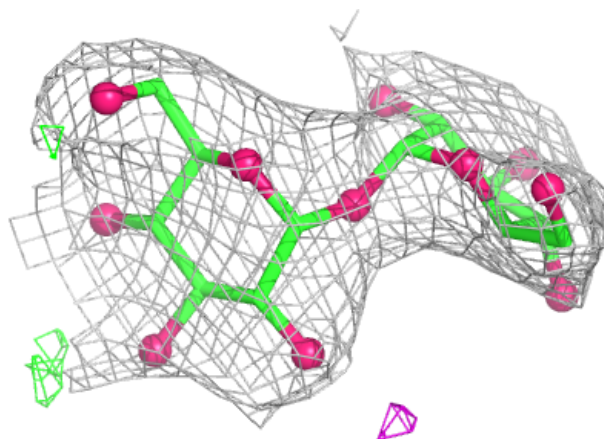
**Electron density around Chain K:**

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



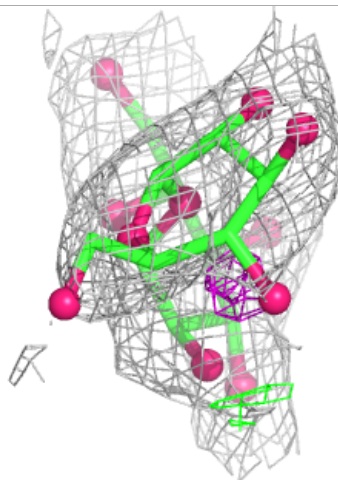
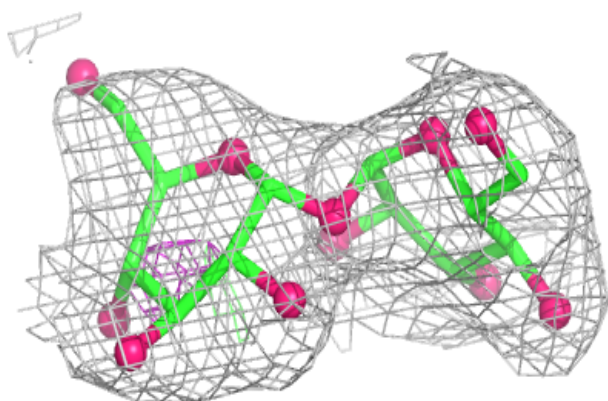
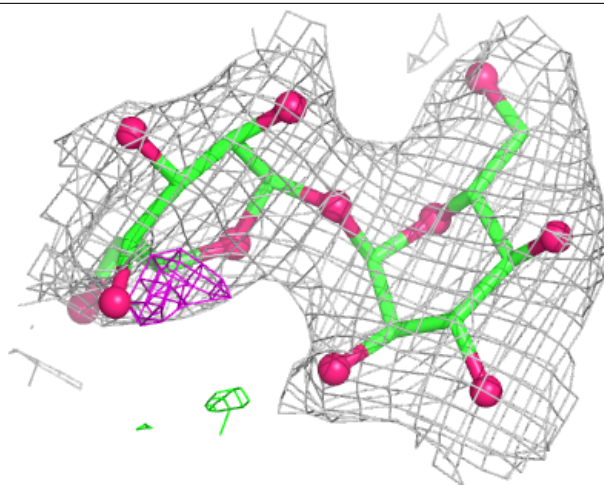
**Electron density around Chain M:**

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



**Electron density around Chain N:**

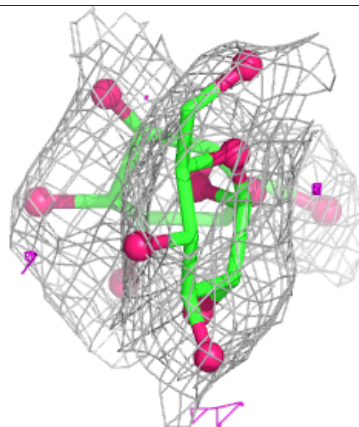
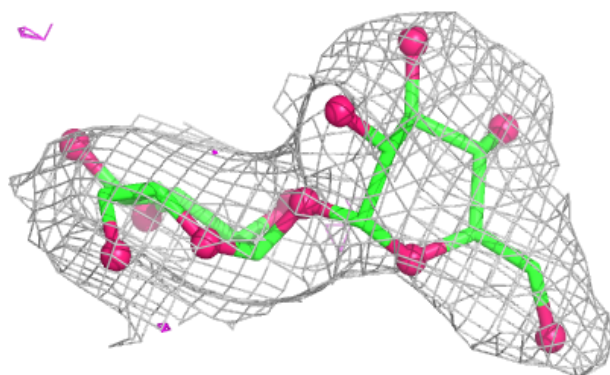
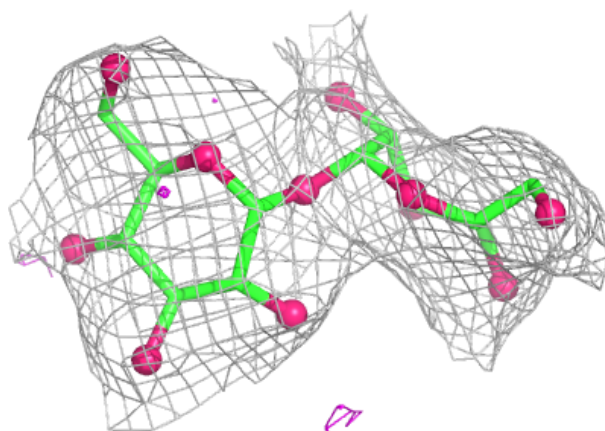
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





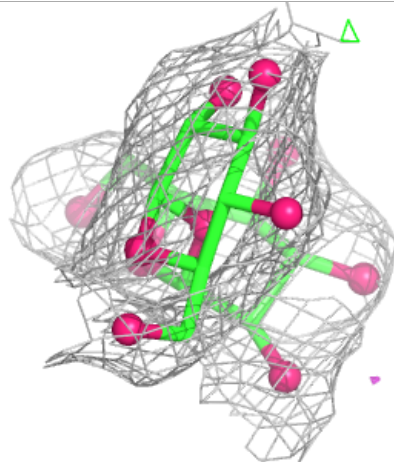
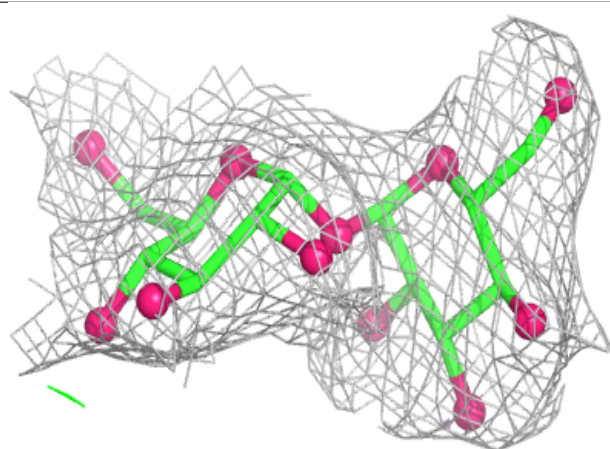
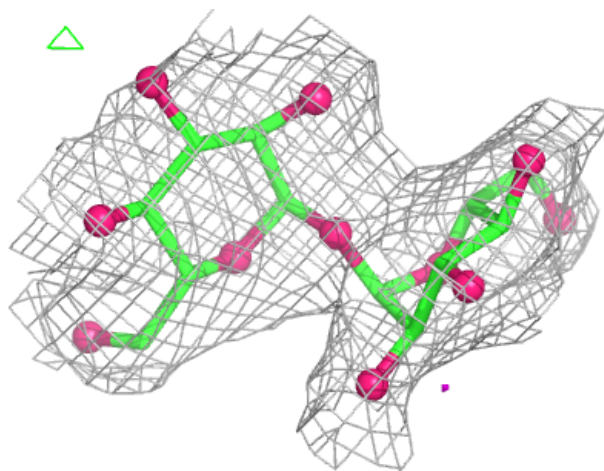
**Electron density around Chain O:**

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



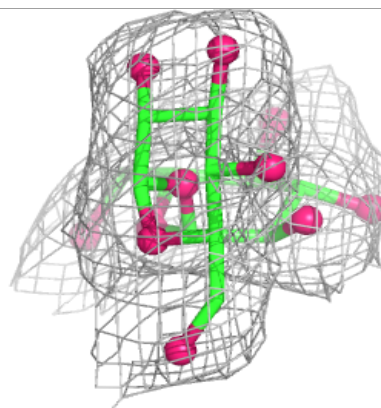
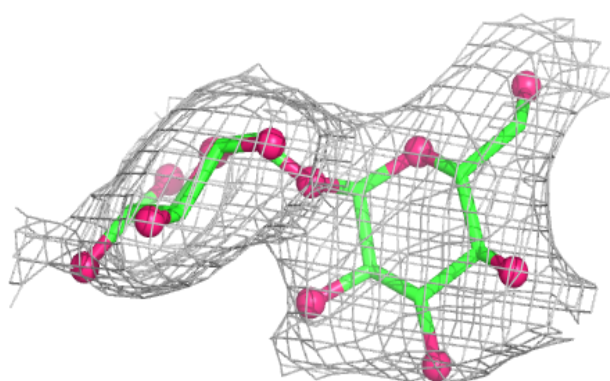
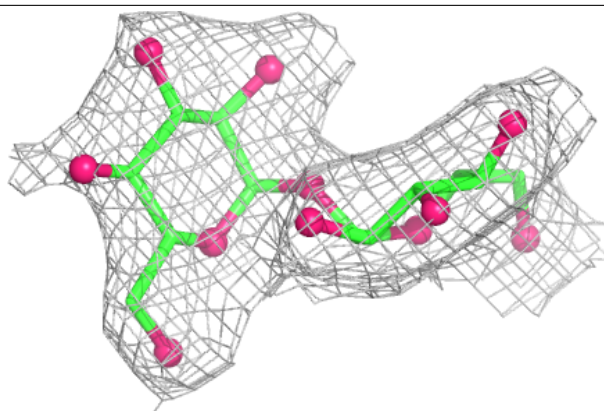
**Electron density around Chain R:**

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

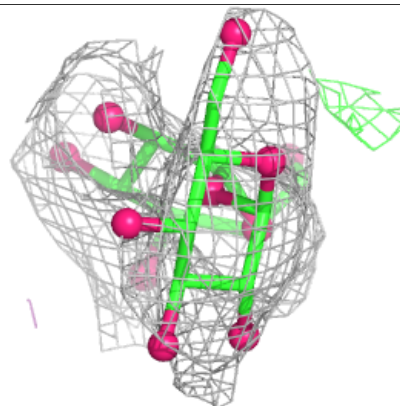
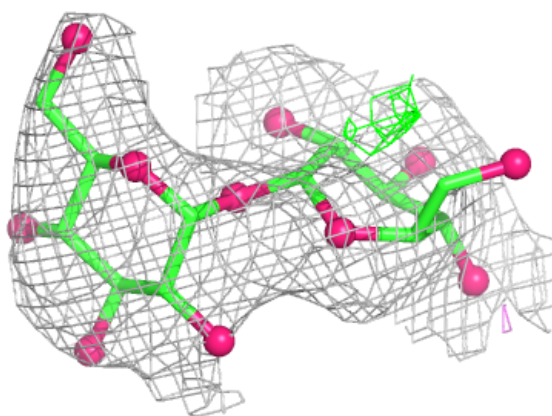


**Electron density around Chain S:**

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

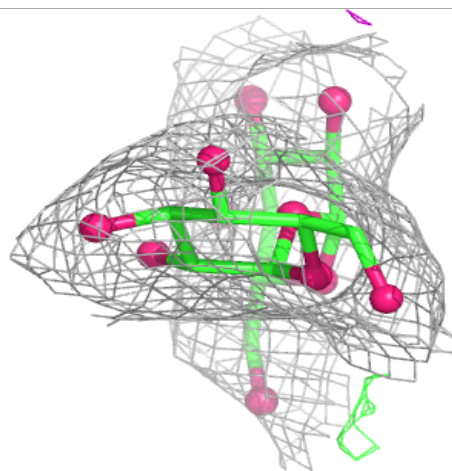
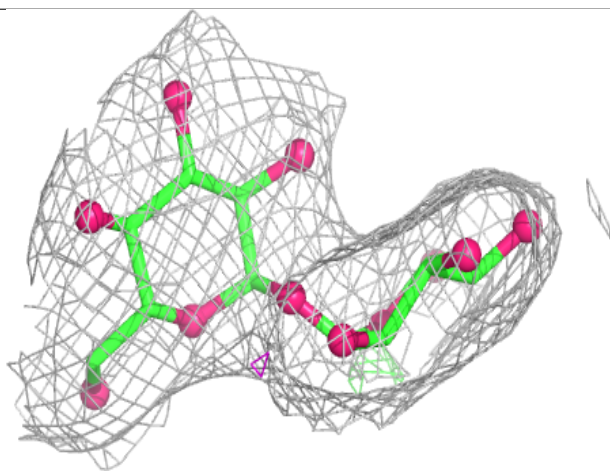
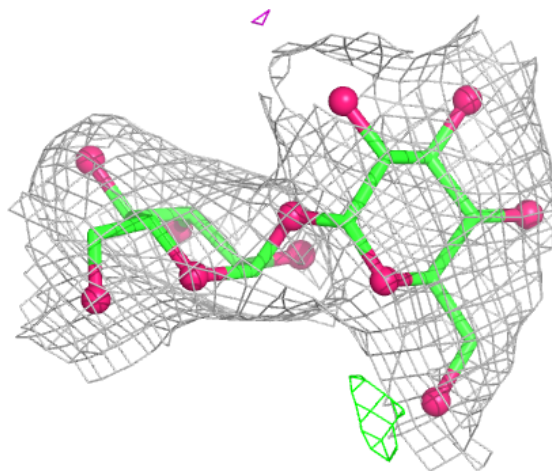
**Electron density around Chain X:**

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

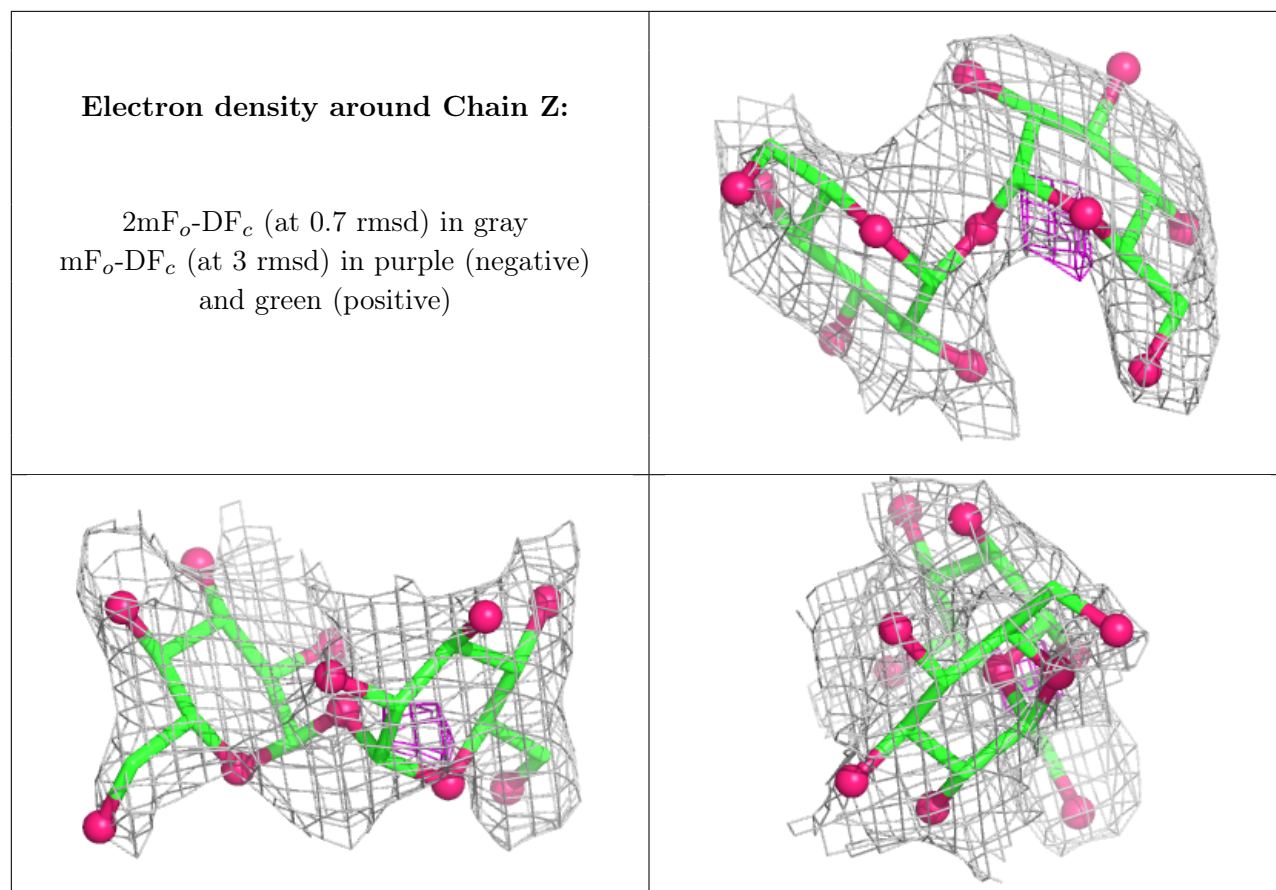


**Electron density around Chain Y:**

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







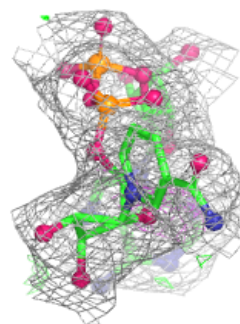
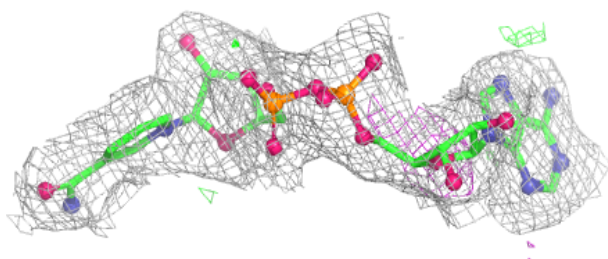
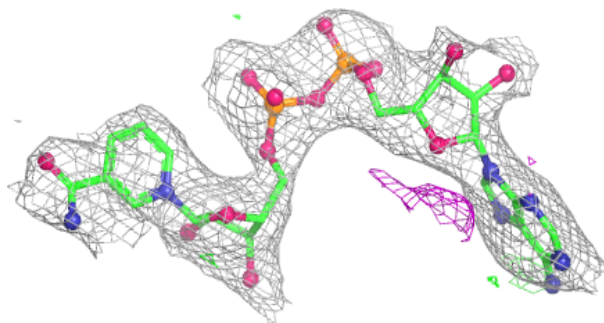
## 6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

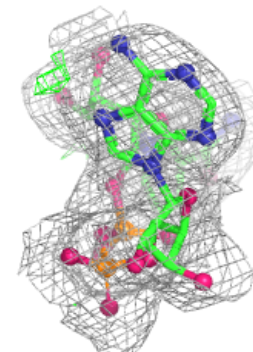
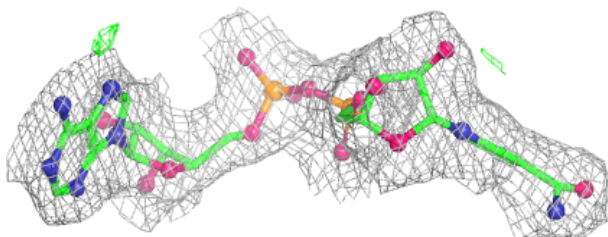
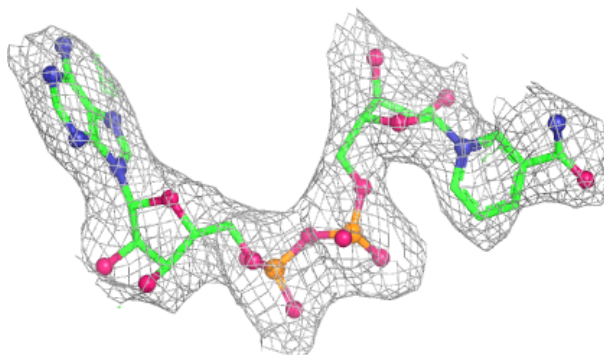
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD 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)

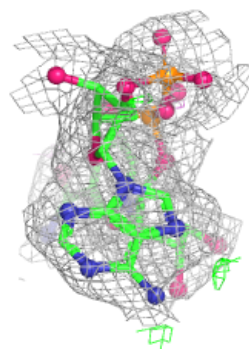
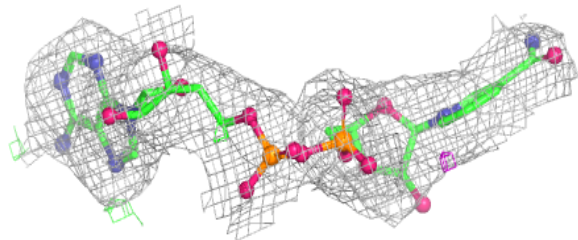
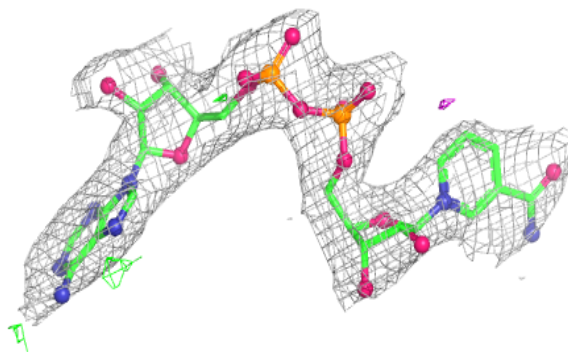
**Electron density around NAD B 501:**

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

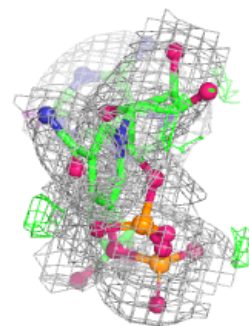
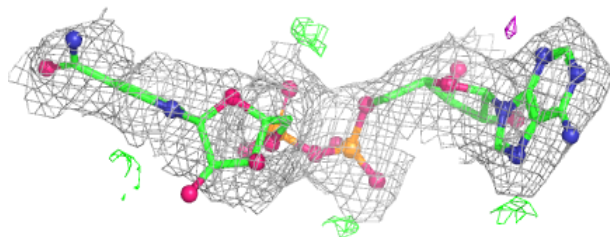
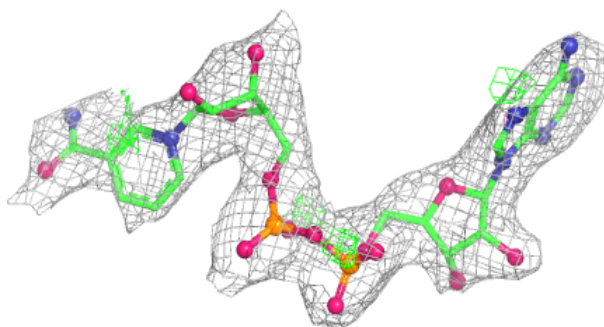


**Electron density around NAD C 501:**

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

**Electron density around NAD D 501:**

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



## 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.