



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:59 AM UTC

PDB ID : 6C01 / pdb\_00006c01  
Title : Human ectonucleotide pyrophosphatase / phosphodiesterase 3 (ENPP3, NPP3, CD203c)  
Authors : Gorelik, A.; Randriamihaja, A.; Illes, K.; Nagar, B.  
Deposited on : 2017-12-27  
Resolution : 2.30 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
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

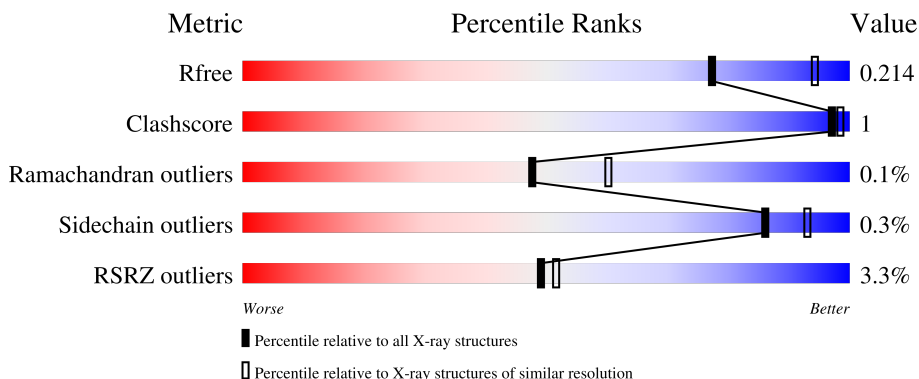
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

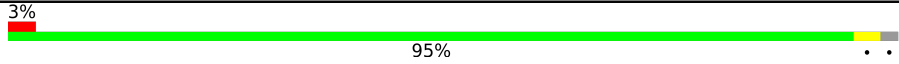
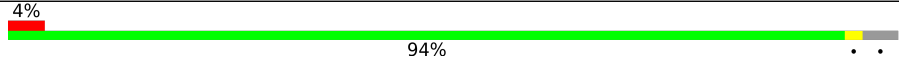
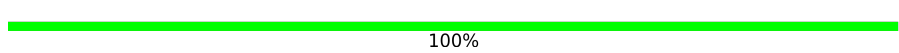
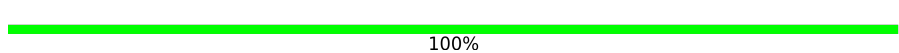

The reported resolution of this entry is 2.30 Å.

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	838	 3% 95%
1	B	838	 4% 94%
2	C	2	 100%
2	K	2	 100%
2	R	2	 100%

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Mol	Chain	Length	Quality of chain
3	D	3	 100%
3	F	3	 100%
3	N	3	 33% 67%
4	E	3	 100%
4	H	3	 100%
4	J	3	 67% 33%
4	M	3	 100%
4	O	3	 100%
4	Q	3	 67% 33%
5	G	5	 80% 20%
6	I	4	 50% 50%
7	L	4	 75% 25%
8	P	5	 60% 40%

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 27890 atoms, of which 13140 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	819	12898	4202	6290	1125	1224	57	0	0	0
1	B	807	12712	4145	6200	1106	1204	57	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

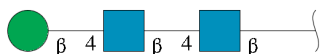
Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ASP	-	expression tag	UNP O14638
A	39	ARG	-	expression tag	UNP O14638
A	40	HIS	-	expression tag	UNP O14638
A	41	HIS	-	expression tag	UNP O14638
A	42	HIS	-	expression tag	UNP O14638
A	43	HIS	-	expression tag	UNP O14638
A	44	HIS	-	expression tag	UNP O14638
A	45	HIS	-	expression tag	UNP O14638
A	46	LYS	-	expression tag	UNP O14638
A	47	LEU	-	expression tag	UNP O14638
B	38	ASP	-	expression tag	UNP O14638
B	39	ARG	-	expression tag	UNP O14638
B	40	HIS	-	expression tag	UNP O14638
B	41	HIS	-	expression tag	UNP O14638
B	42	HIS	-	expression tag	UNP O14638
B	43	HIS	-	expression tag	UNP O14638
B	44	HIS	-	expression tag	UNP O14638
B	45	HIS	-	expression tag	UNP O14638
B	46	LYS	-	expression tag	UNP O14638
B	47	LEU	-	expression tag	UNP O14638

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



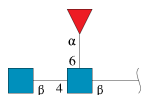
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	C	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	K	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	R	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	D	3	Total	C	H	N	O	0	0	0
			76	22	37	2	15			
3	F	3	Total	C	H	N	O	0	0	0
			76	22	37	2	15			
3	N	3	Total	C	H	N	O	0	0	0
			76	22	37	2	15			

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



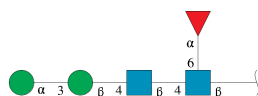
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	E	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			
4	H	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			
4	J	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			
4	M	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	O	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			
4	Q	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acet amido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
5	G	5	Total	C	H	N	O	0	0	0
			117	34	57	2	24			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc o pyranose.



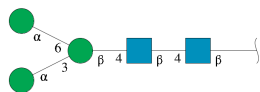
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
6	I	4	Total	C	H	N	O	0	0	0
			97	28	47	2	20			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc o pyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
7	L	4	Total	C	H	N	O	0	0	0
			97	28	47	2	20			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
8	P	5	118	34	57	2	25	0	0	0

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
9	A	2	2	2	0	0
9	B	2	2	2	0	0

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
10	A	1	1	1	0	0
10	B	1	1	1	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
11	A	1	28	8	14	1	5	0	0
11	B	1	28	8	14	1	5	0	0

- Molecule 12 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
12	A	1	1	1	0	0
12	B	1	1	1	0	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	527	527	527	0	0
13	B	417	417	417	0	0



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

Chain R:  100%

MAG1  
MAG2

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

Chain D:  100%

MAG1  
MAG2  
BMA3

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

Chain F:  100%

MAG1  
MAG2  
BMA3

- Molecule 3: 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%

MAG1  
MAG2  
BMA3

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

Chain E:  100%

MAG1  
MAG2  
FUC3

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

Chain H:  100%

MAG1  
MAG2  
FUC3

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

Chain J:  67% 33%



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

Chain M: 100%



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

Chain O: 100%



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

Chain Q: 67% 33%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 80% 20%



- Molecule 6: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 50% 50%



- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 75% 25%



- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  60% 40%

MAG1	MAG2	EMG3	MAN4	MAN5
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.18Å 133.64Å 167.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.27 – 2.30 48.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (48.27-2.30) 83.3 (48.27-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.174 , 0.214 0.177 , 0.214	Depositor DCC
$R_{free}$ test set	1918 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	27890	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.99 % 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 6.8911e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: BMA, NA, NAG, FUC, CA, MAN, ZN

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	0.21	0/6806	0.36	0/9255
1	B	0.19	0/6707	0.35	0/9119
All	All	0.20	0/13513	0.36	0/18374

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6608	6290	6290	13	1
1	B	6512	6200	6199	11	0
2	C	28	27	25	0	0
2	K	28	27	25	0	0
2	R	28	27	25	0	0
3	D	39	37	34	0	0
3	F	39	37	34	0	0
3	N	39	37	34	0	0
4	E	38	37	34	0	0
4	H	38	37	34	0	0
4	J	38	37	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	38	37	34	0	0
4	O	38	37	34	0	0
4	Q	38	37	34	0	0
5	G	60	57	52	0	0
6	I	50	47	43	0	0
7	L	50	47	43	0	0
8	P	61	57	52	0	1
9	A	2	0	0	0	0
9	B	2	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	14	14	13	0	0
11	B	14	14	13	1	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
13	A	527	0	0	3	1
13	B	417	0	0	3	1
All	All	14750	13140	13086	25	2

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 1.

The worst 5 of 25 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:NH2	13:A:1001:HOH:O	2.18	0.76
1:B:102:ARG:NH2	1:B:115:CYS:SG	2.60	0.73
1:B:170:ARG:NH2	13:B:1002:HOH:O	2.23	0.70
1:A:225:ASP:OD1	1:A:226:ASN:N	2.34	0.59
1:A:195:LYS:NZ	1:A:510:GLU:OE1	2.40	0.54

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:SER:O	8:P:5:MAN:O6[4_566]	2.08	0.12
13:A:1321:HOH:O	13:B:1126:HOH:O[4_476]	2.09	0.11

## 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	817/838 (98%)	793 (97%)	23 (3%)	1 (0%)	48	60
1	B	801/838 (96%)	773 (96%)	28 (4%)	0	100	100
All	All	1618/1676 (96%)	1566 (97%)	51 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	662	PRO

### 5.3.2 Protein sidechains [i](#)

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	740/758 (98%)	738 (100%)	2 (0%)	86	93
1	B	730/758 (96%)	728 (100%)	2 (0%)	86	93
All	All	1470/1516 (97%)	1466 (100%)	4 (0%)	86	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	MET
1	A	808	ILE
1	B	228	MET
1	B	284	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	744	ASN
1	B	134	GLN
1	B	528	GLN
1	B	245	ASN
1	B	465	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

51 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	C	1	1,2	14,14,15	0.30	0	17,19,21	0.60	0
2	NAG	C	2	2	14,14,15	0.24	0	17,19,21	0.52	0
3	NAG	D	1	3,1	14,14,15	0.38	0	17,19,21	0.50	0
3	NAG	D	2	3	14,14,15	0.49	0	17,19,21	0.51	0
3	BMA	D	3	3	11,11,12	0.91	0	15,15,17	0.72	0
4	NAG	E	1	1,4	14,14,15	0.32	0	17,19,21	0.60	0
4	NAG	E	2	4	14,14,15	0.44	0	17,19,21	0.41	0
4	FUC	E	3	4	10,10,11	0.86	0	14,14,16	0.78	0
3	NAG	F	1	3,1	14,14,15	0.19	0	17,19,21	0.70	0
3	NAG	F	2	3	14,14,15	0.47	0	17,19,21	0.47	0
3	BMA	F	3	3	11,11,12	0.74	0	15,15,17	0.65	0
5	NAG	G	1	1,5	14,14,15	0.27	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	G	2	5	14,14,15	0.26	0	17,19,21	0.40	0
5	BMA	G	3	5	11,11,12	0.63	0	15,15,17	0.86	0
5	MAN	G	4	5	11,11,12	0.95	0	15,15,17	1.19	1 (6%)
5	FUC	G	5	5	10,10,11	0.59	0	14,14,16	0.65	0
4	NAG	H	1	1,4	14,14,15	0.39	0	17,19,21	0.59	0
4	NAG	H	2	4	14,14,15	0.24	0	17,19,21	0.50	0
4	FUC	H	3	4	10,10,11	0.79	0	14,14,16	0.70	0
6	NAG	I	1	1,6	14,14,15	0.45	0	17,19,21	0.50	0
6	NAG	I	2	6	14,14,15	0.24	0	17,19,21	0.52	0
6	BMA	I	3	6	11,11,12	1.07	1 (9%)	15,15,17	0.74	0
6	MAN	I	4	6	11,11,12	1.11	0	15,15,17	1.10	2 (13%)
4	NAG	J	1	1,4	14,14,15	0.36	0	17,19,21	0.39	0
4	NAG	J	2	4	14,14,15	0.27	0	17,19,21	0.48	0
4	FUC	J	3	4	10,10,11	1.38	2 (20%)	14,14,16	1.21	1 (7%)
2	NAG	K	1	1,2	14,14,15	0.21	0	17,19,21	0.53	0
2	NAG	K	2	2	14,14,15	0.23	0	17,19,21	0.60	0
7	NAG	L	1	7,1	14,14,15	0.28	0	17,19,21	0.51	0
7	NAG	L	2	7	14,14,15	0.37	0	17,19,21	0.44	0
7	BMA	L	3	7	11,11,12	0.79	0	15,15,17	0.65	0
7	MAN	L	4	7	11,11,12	0.87	0	15,15,17	1.18	1 (6%)
4	NAG	M	1	1,4	14,14,15	0.31	0	17,19,21	0.47	0
4	NAG	M	2	4	14,14,15	0.27	0	17,19,21	0.67	0
4	FUC	M	3	4	10,10,11	0.86	0	14,14,16	0.76	0
3	NAG	N	1	3,1	14,14,15	0.31	0	17,19,21	0.64	0
3	NAG	N	2	3	14,14,15	0.57	1 (7%)	17,19,21	0.75	0
3	BMA	N	3	3	11,11,12	1.09	1 (9%)	15,15,17	0.86	1 (6%)
4	NAG	O	1	1,4	14,14,15	0.34	0	17,19,21	0.56	0
4	NAG	O	2	4	14,14,15	0.36	0	17,19,21	0.40	0
4	FUC	O	3	4	10,10,11	0.55	0	14,14,16	0.79	0
8	NAG	P	1	8,1	14,14,15	0.38	0	17,19,21	0.50	0
8	NAG	P	2	8	14,14,15	0.17	0	17,19,21	0.52	0
8	BMA	P	3	8	11,11,12	0.42	0	15,15,17	0.70	0
8	MAN	P	4	8	11,11,12	0.85	0	15,15,17	1.05	1 (6%)
8	MAN	P	5	8	11,11,12	0.92	0	15,15,17	0.80	0
4	NAG	Q	1	1,4	14,14,15	0.31	0	17,19,21	0.45	0
4	NAG	Q	2	4	14,14,15	0.40	0	17,19,21	0.50	0
4	FUC	Q	3	4	10,10,11	0.74	0	14,14,16	0.87	1 (7%)
2	NAG	R	1	1,2	14,14,15	0.40	0	17,19,21	0.78	0
2	NAG	R	2	2	14,14,15	0.33	0	17,19,21	0.41	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. '2' means no outliers of that kind were identified.

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	N	3	3	-	2/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	O	2	4	-	3/6/23/26	0/1/1/1
4	FUC	O	3	4	-	-	0/1/1/1
8	NAG	P	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	P	2	8	-	0/6/23/26	0/1/1/1
8	BMA	P	3	8	-	0/2/19/22	0/1/1/1
8	MAN	P	4	8	-	1/2/19/22	0/1/1/1
8	MAN	P	5	8	-	2/2/19/22	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
4	FUC	Q	3	4	-	-	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	FUC	C1-C2	3.66	1.61	1.52
6	I	3	BMA	C1-C2	2.48	1.58	1.52
3	N	3	BMA	C4-C5	2.33	1.58	1.53
4	J	3	FUC	C2-C3	2.06	1.55	1.52
3	N	2	NAG	O5-C1	-2.03	1.40	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	4	MAN	C1-O5-C5	3.76	117.23	112.19
4	J	3	FUC	C1-C2-C3	3.56	114.83	109.64
7	L	4	MAN	C1-O5-C5	3.54	116.93	112.19
8	P	4	MAN	C1-O5-C5	2.90	116.07	112.19
4	Q	3	FUC	C1-C2-C3	2.40	113.14	109.64

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	3	BMA	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
8	P	5	MAN	O5-C5-C6-O6

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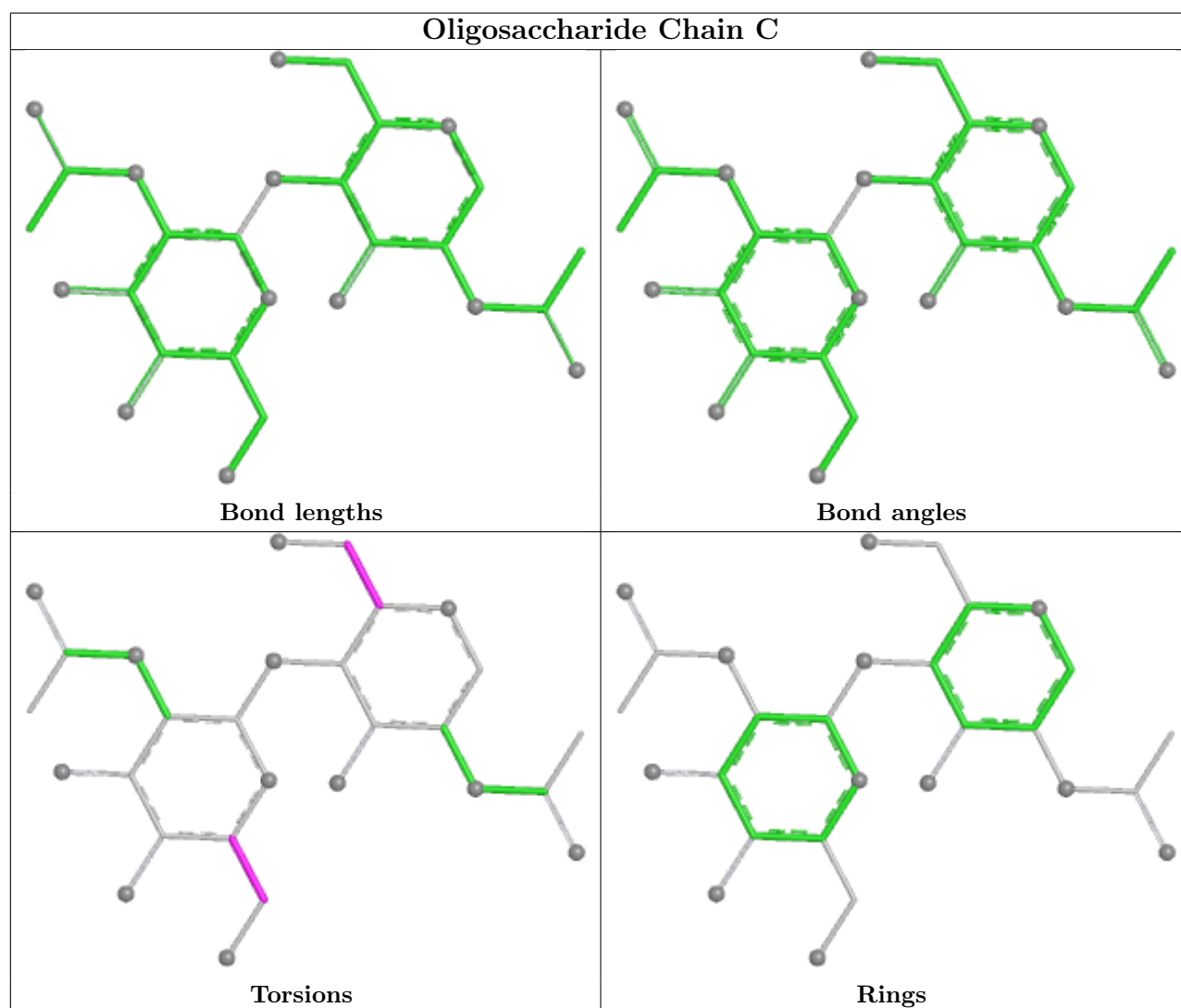
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6

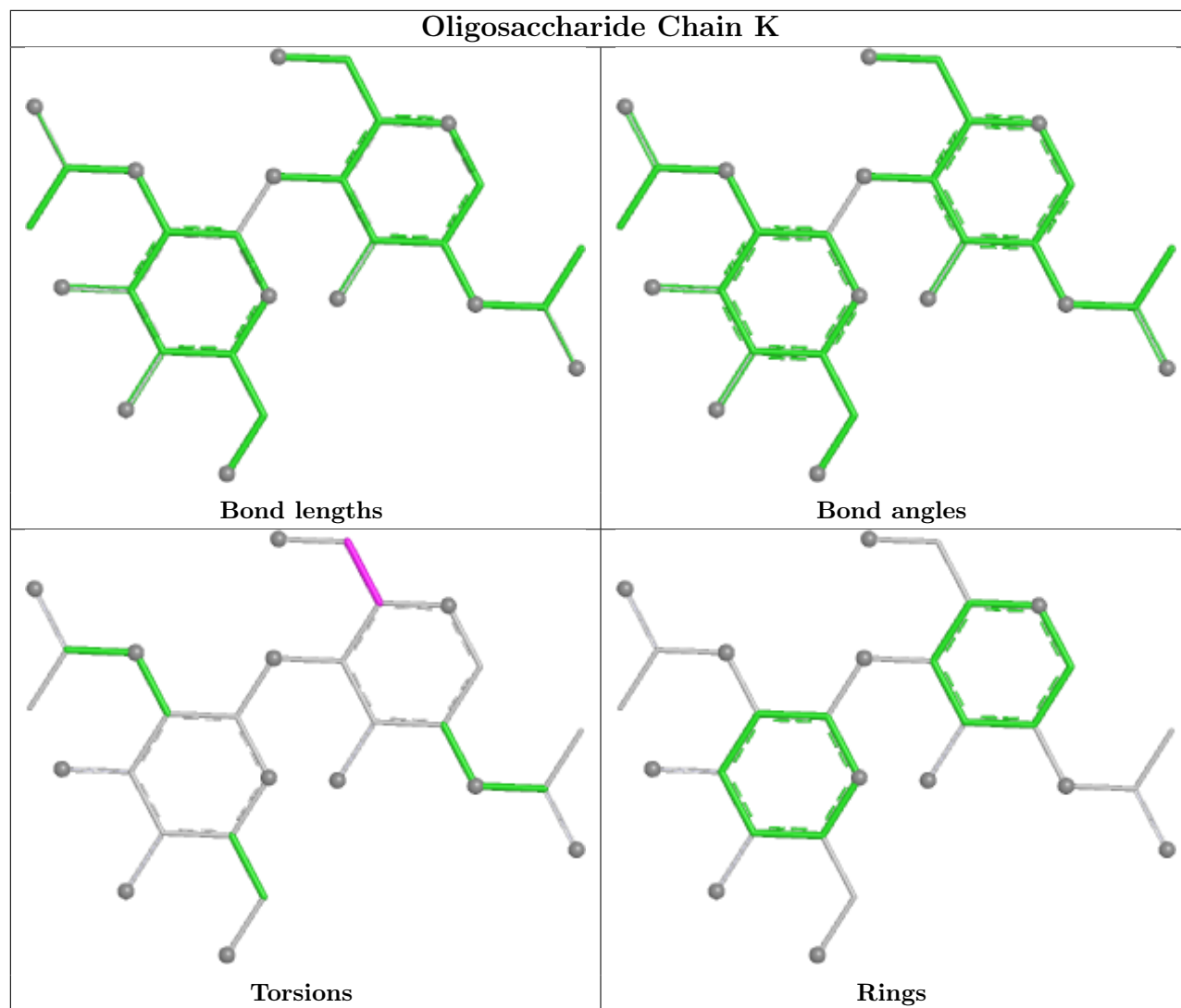
There are no ring outliers.

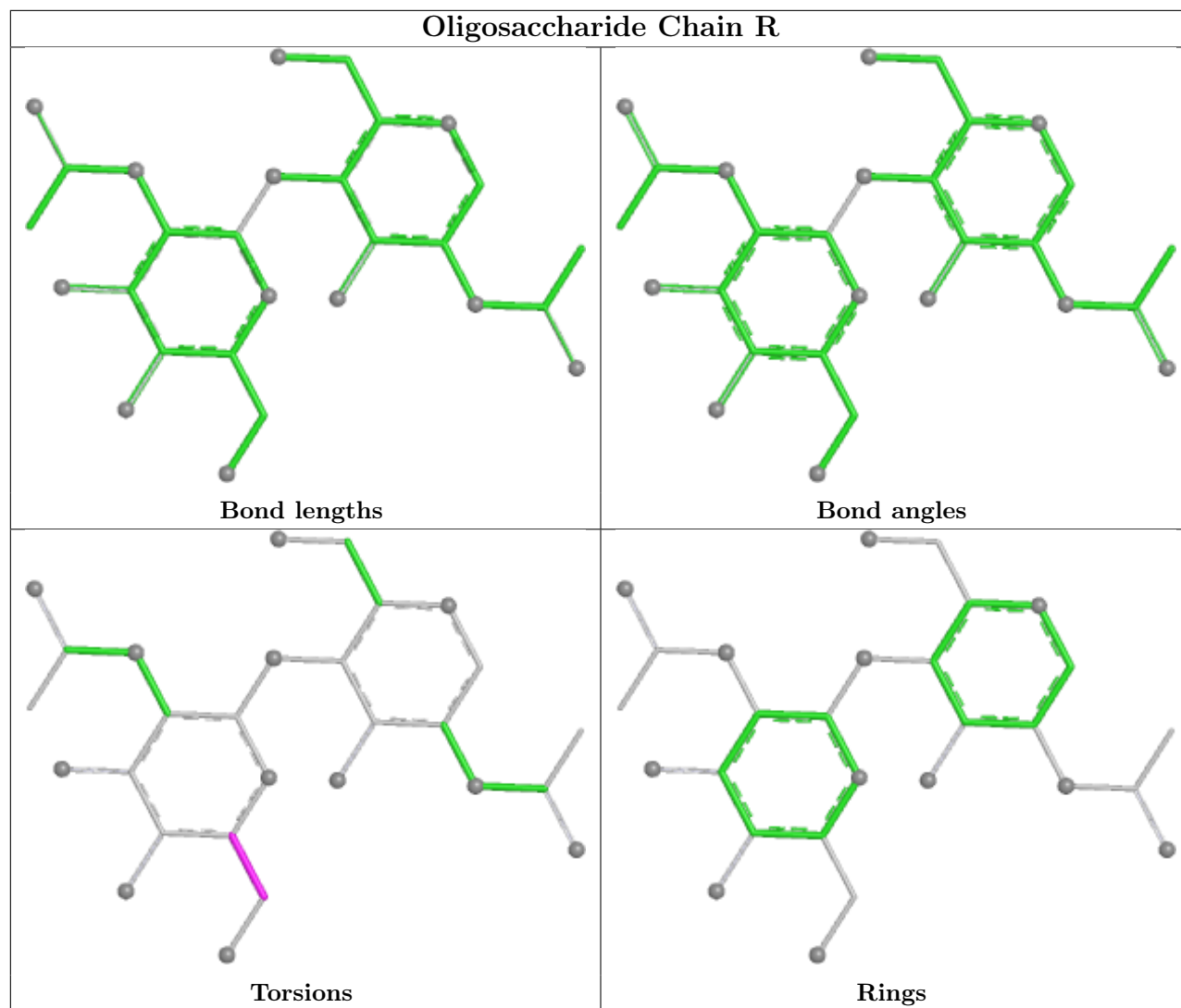
1 monomer is involved in 1 short contact:

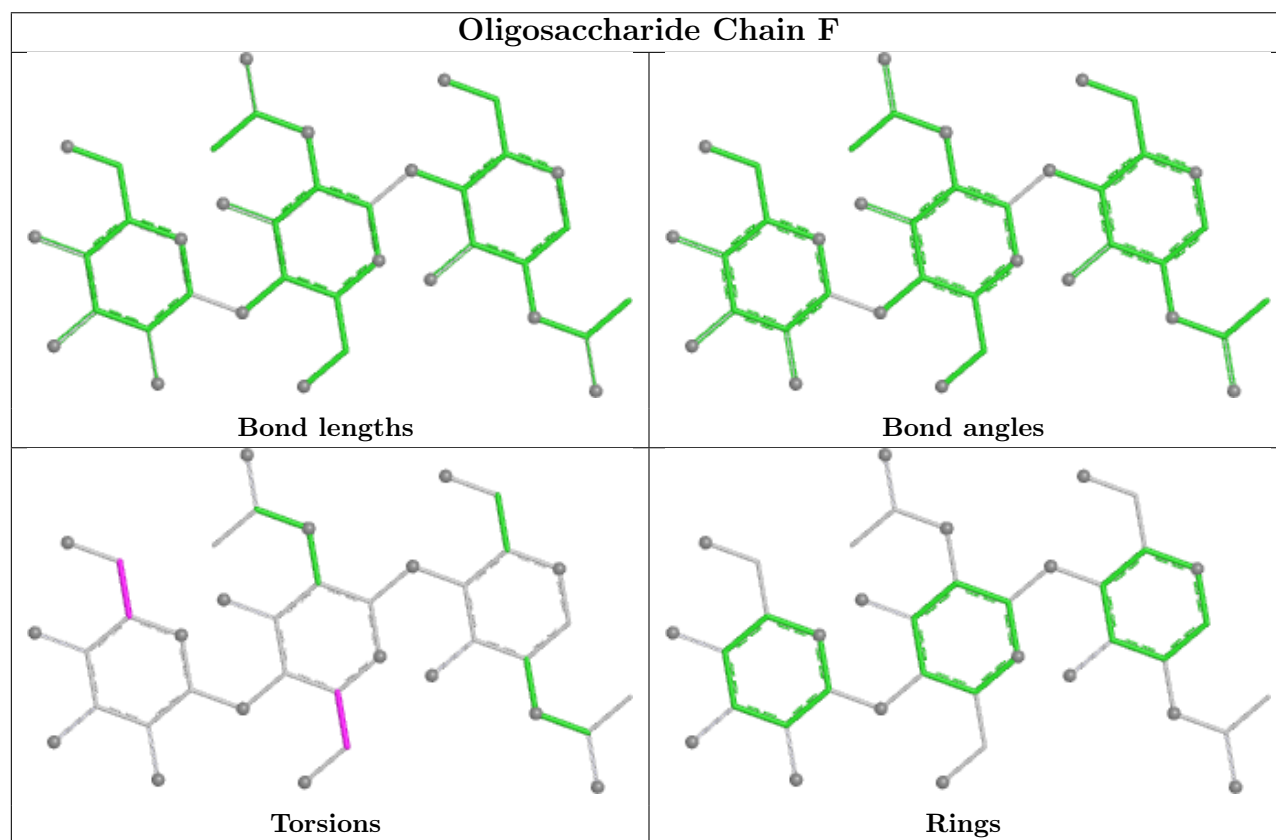
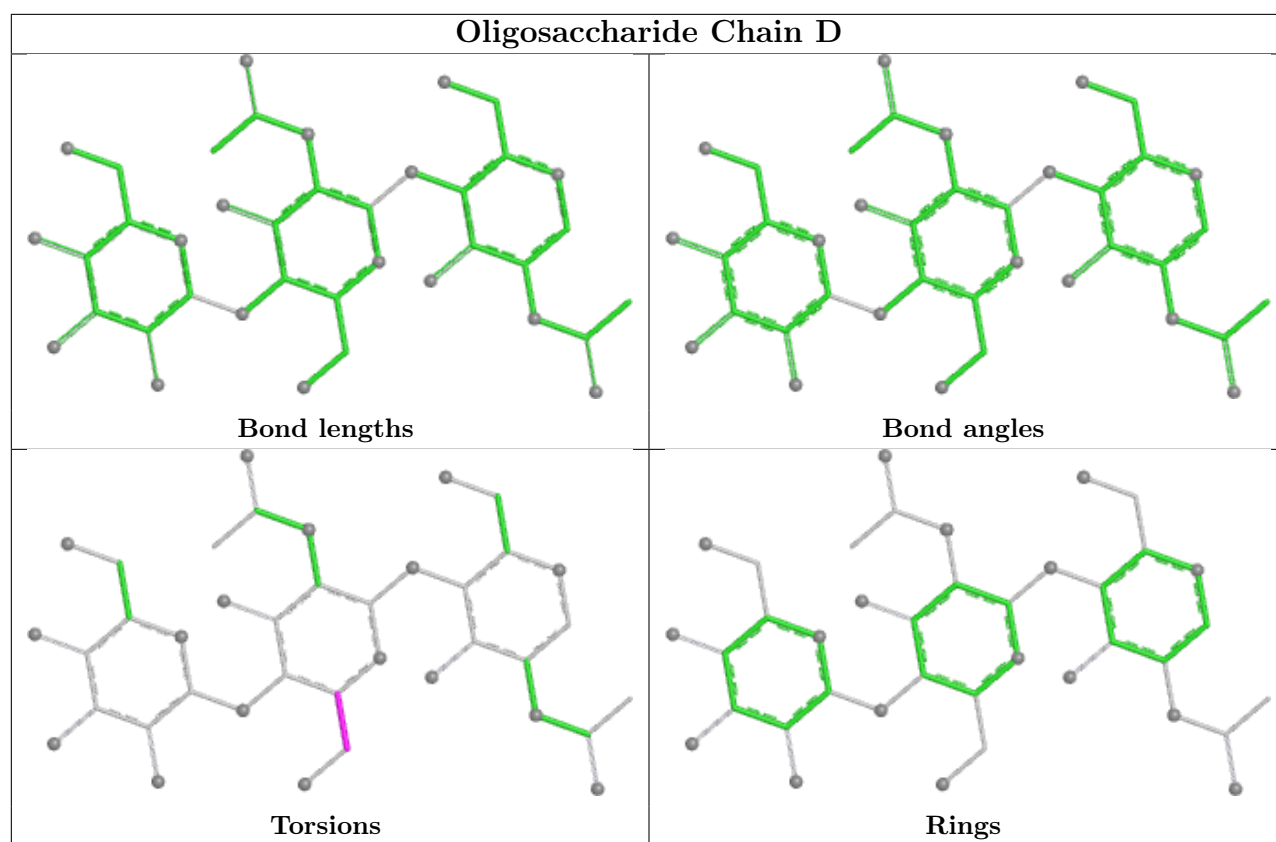
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	P	5	MAN	0	1

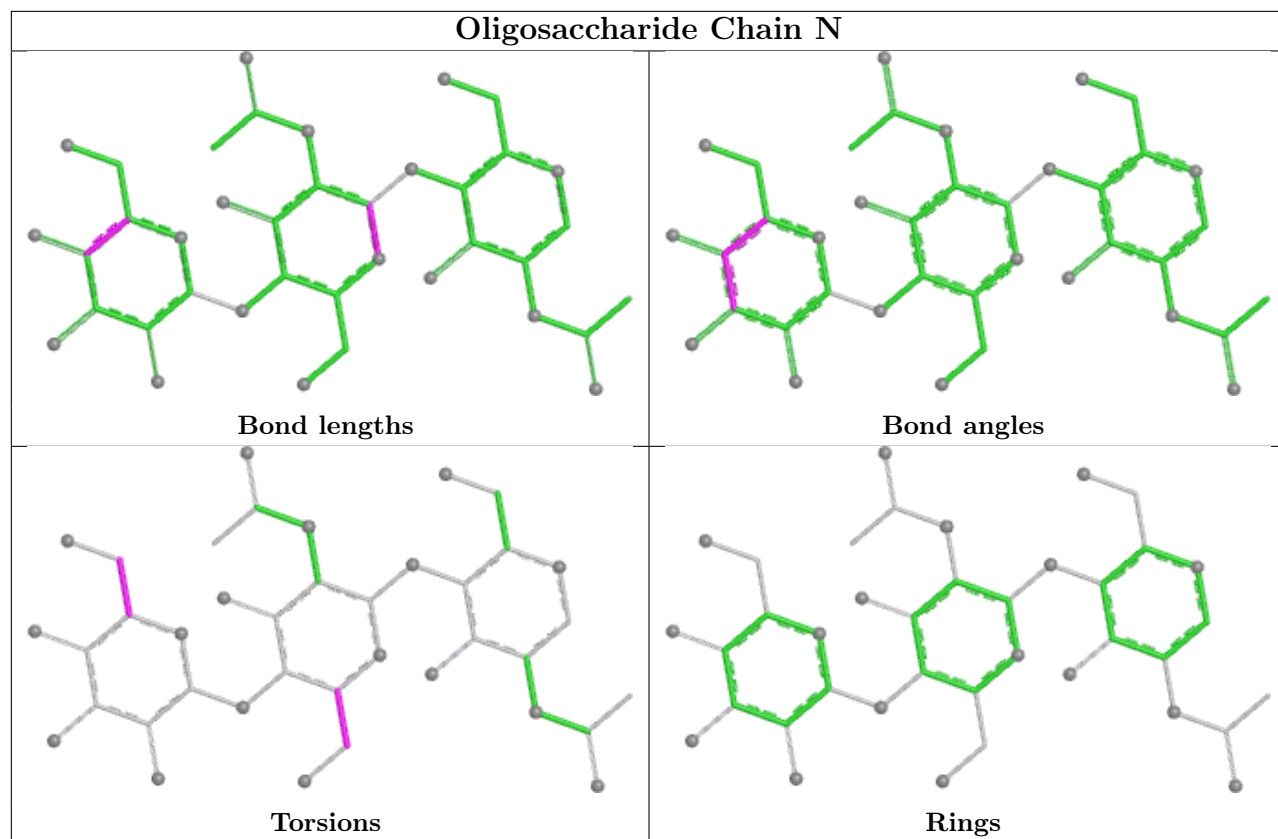
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

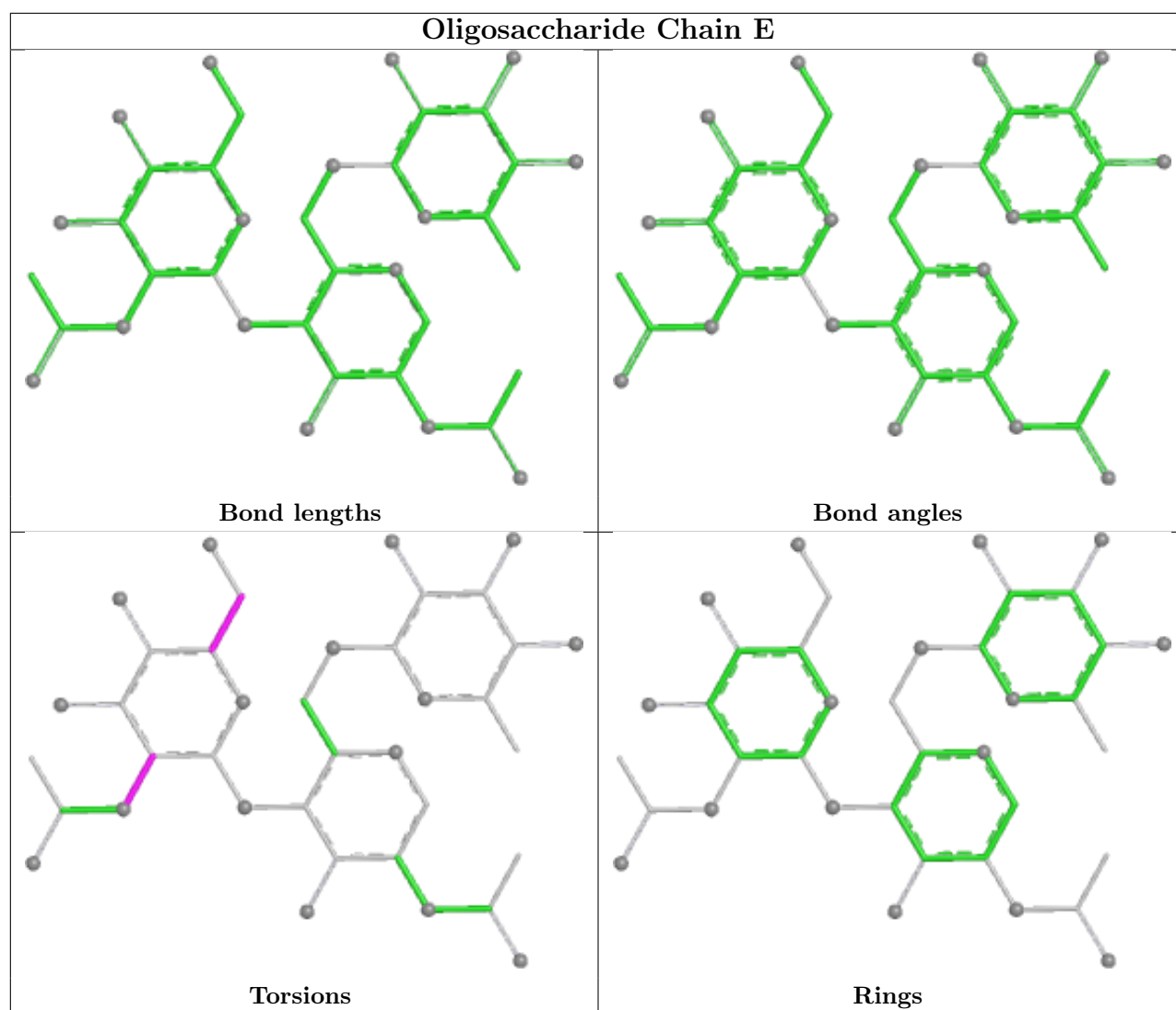


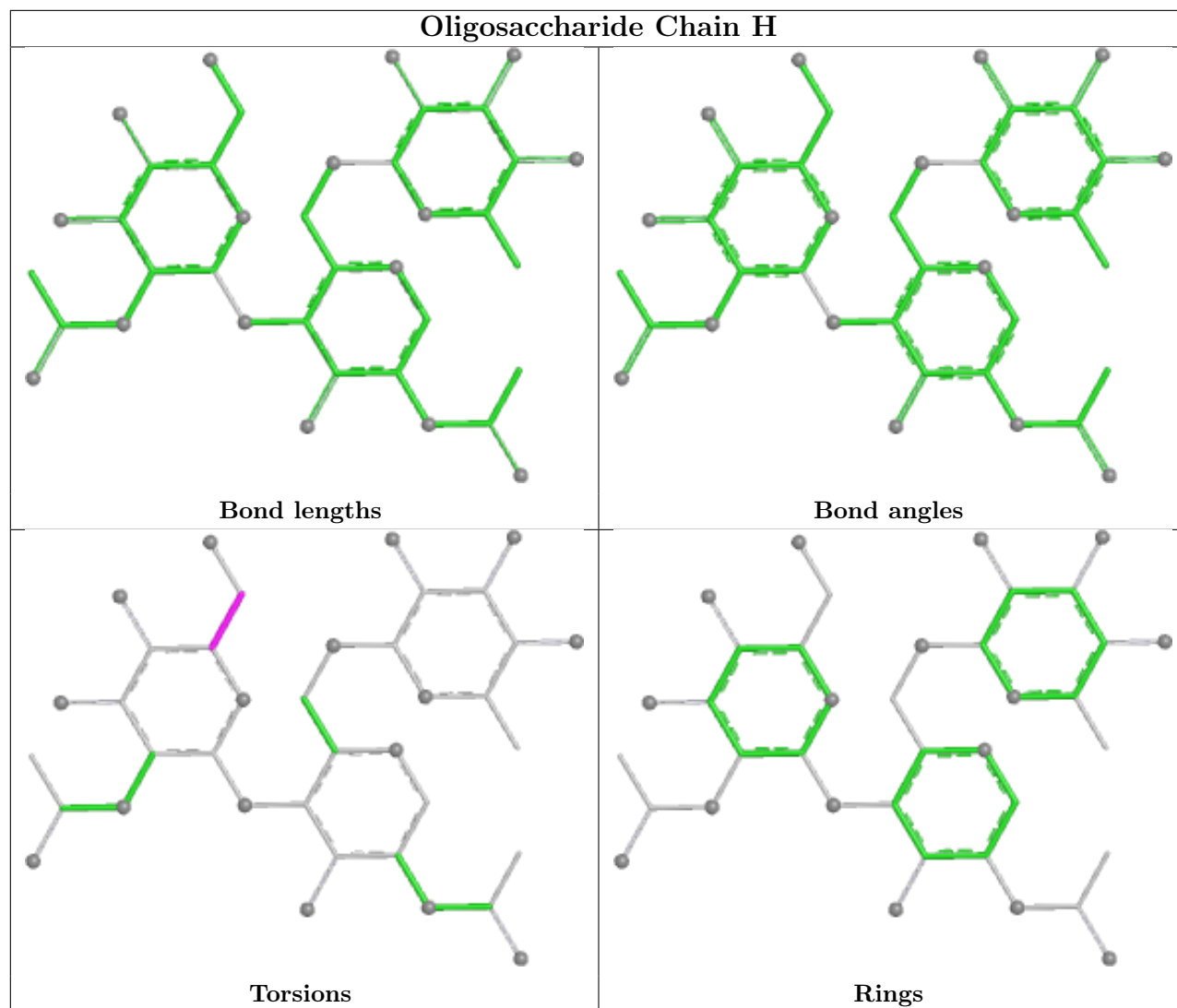


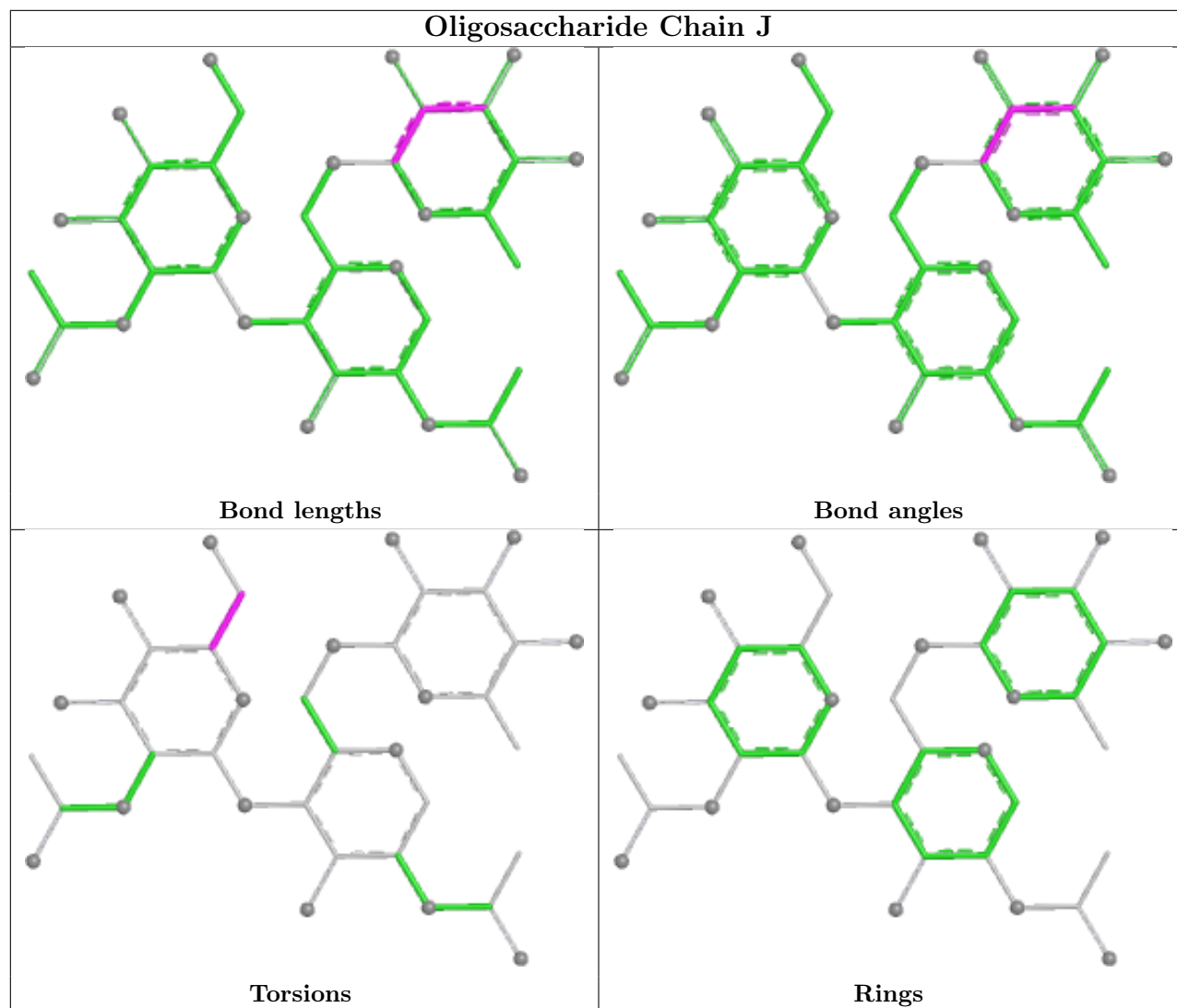


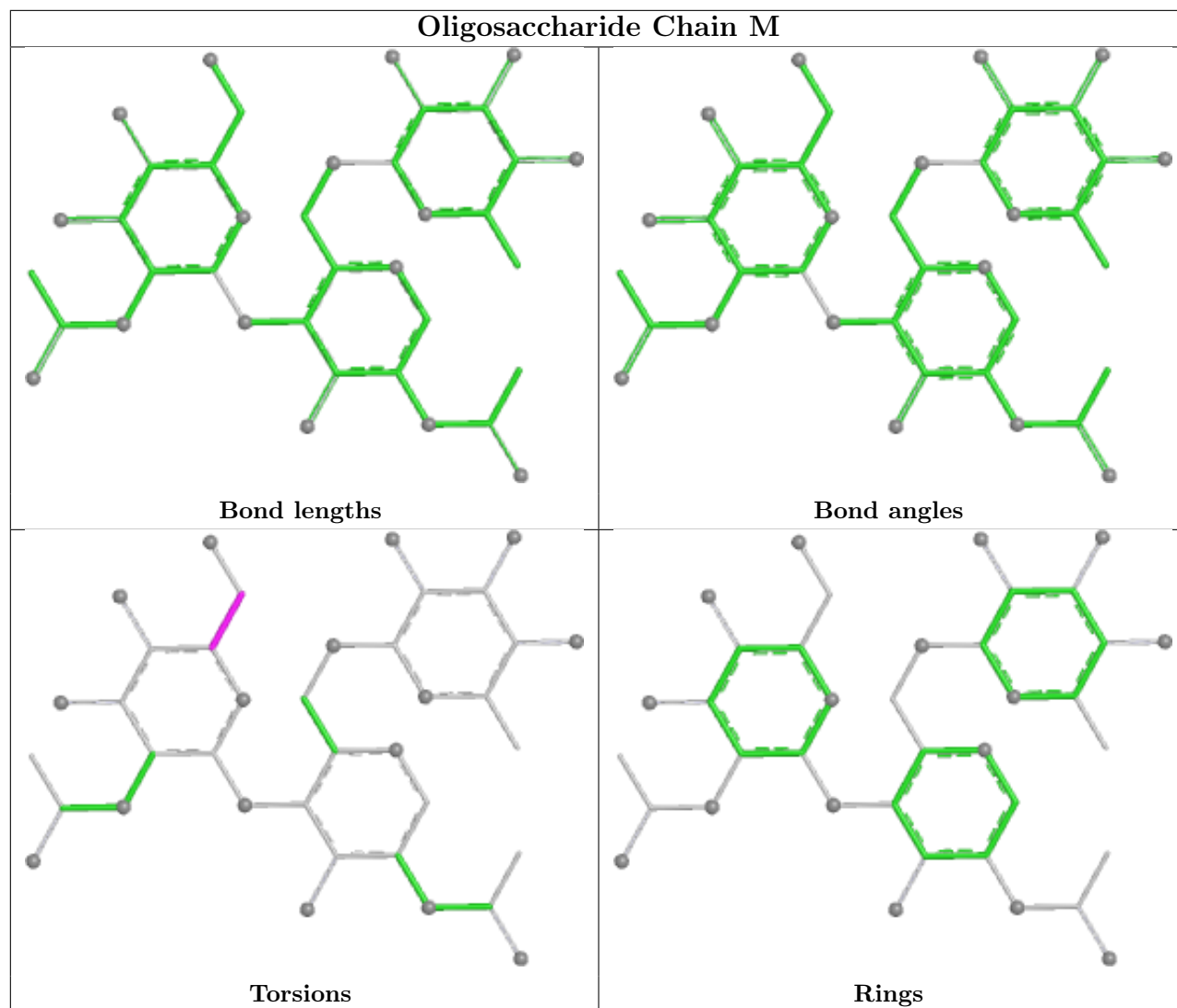


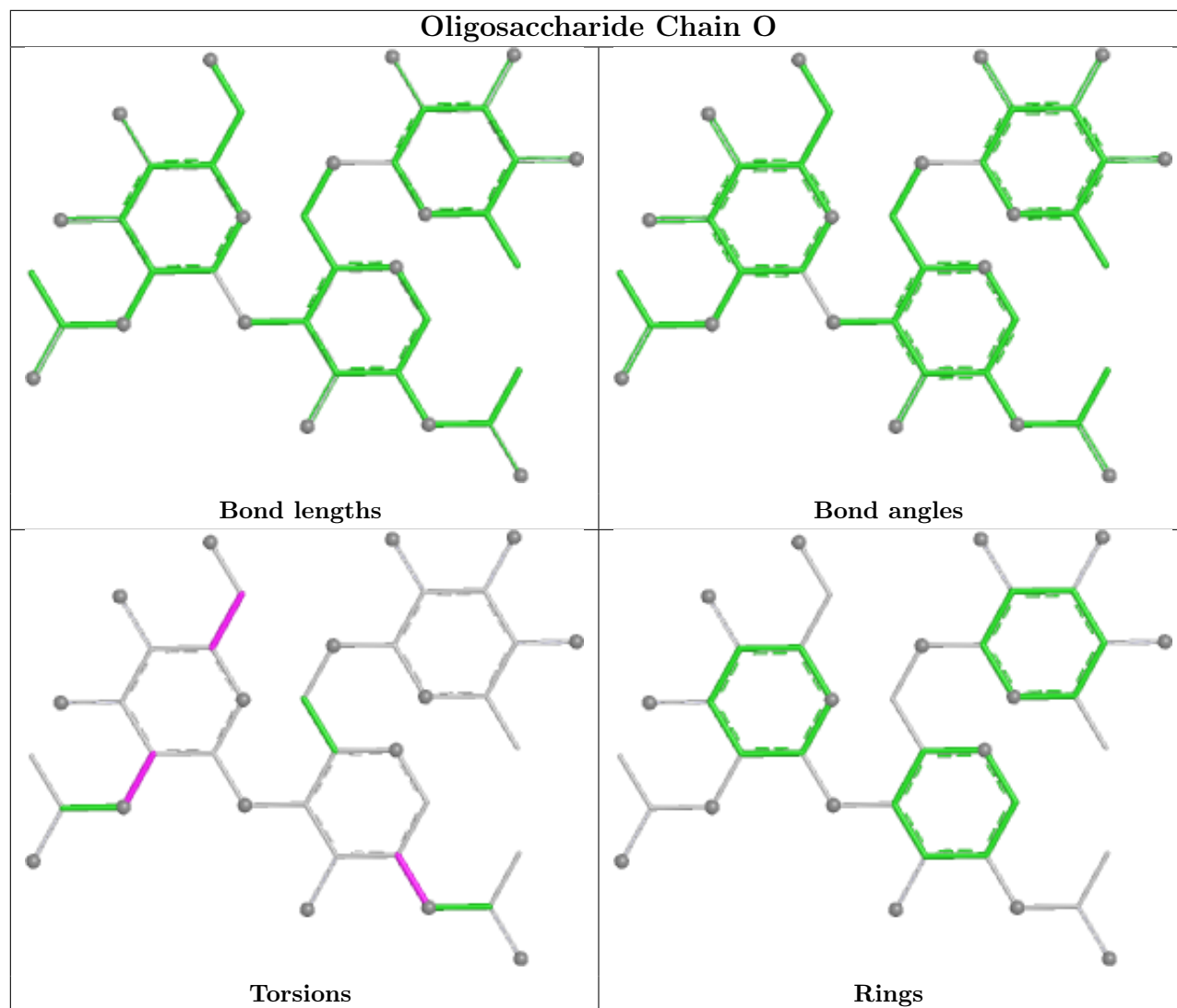


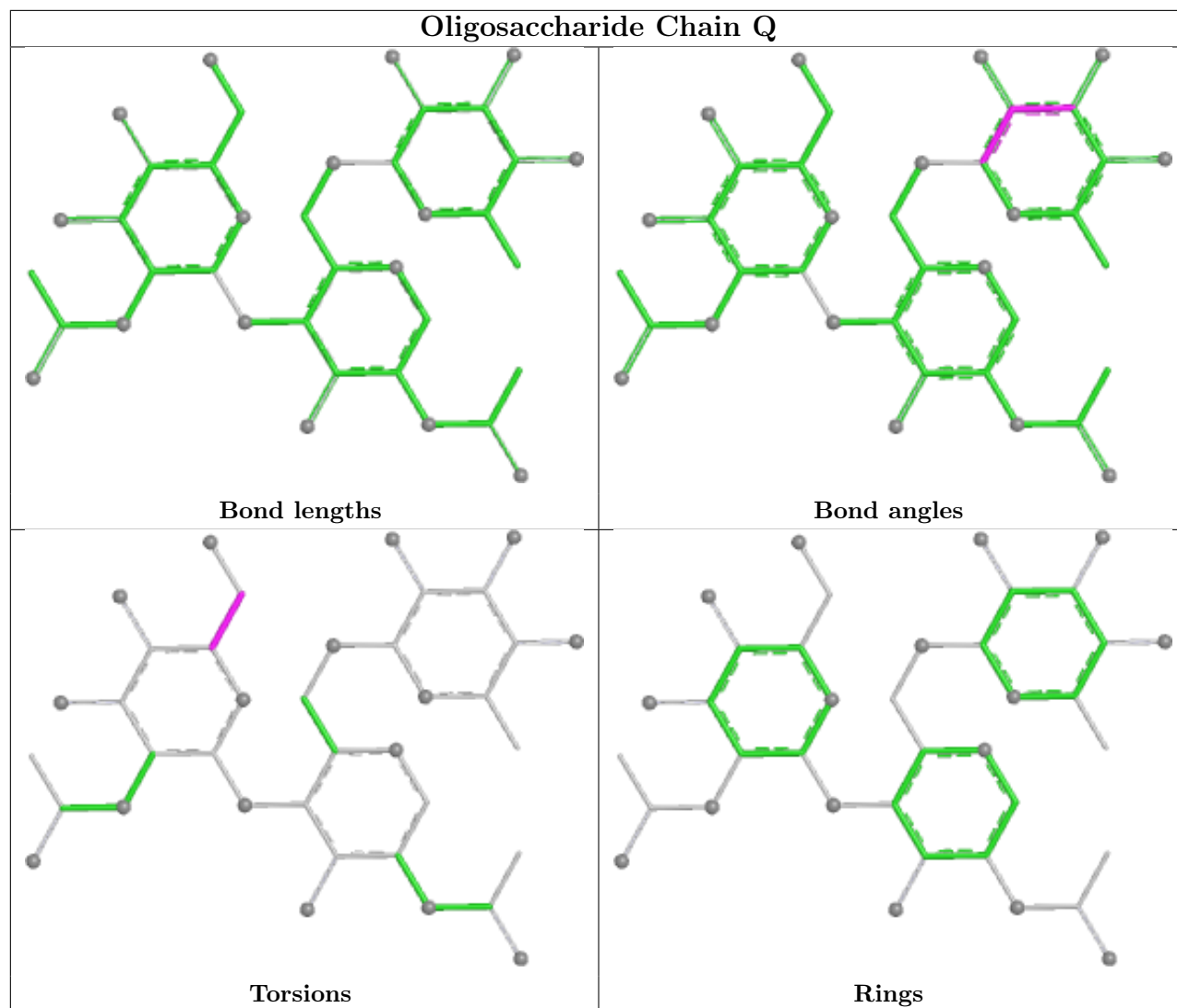


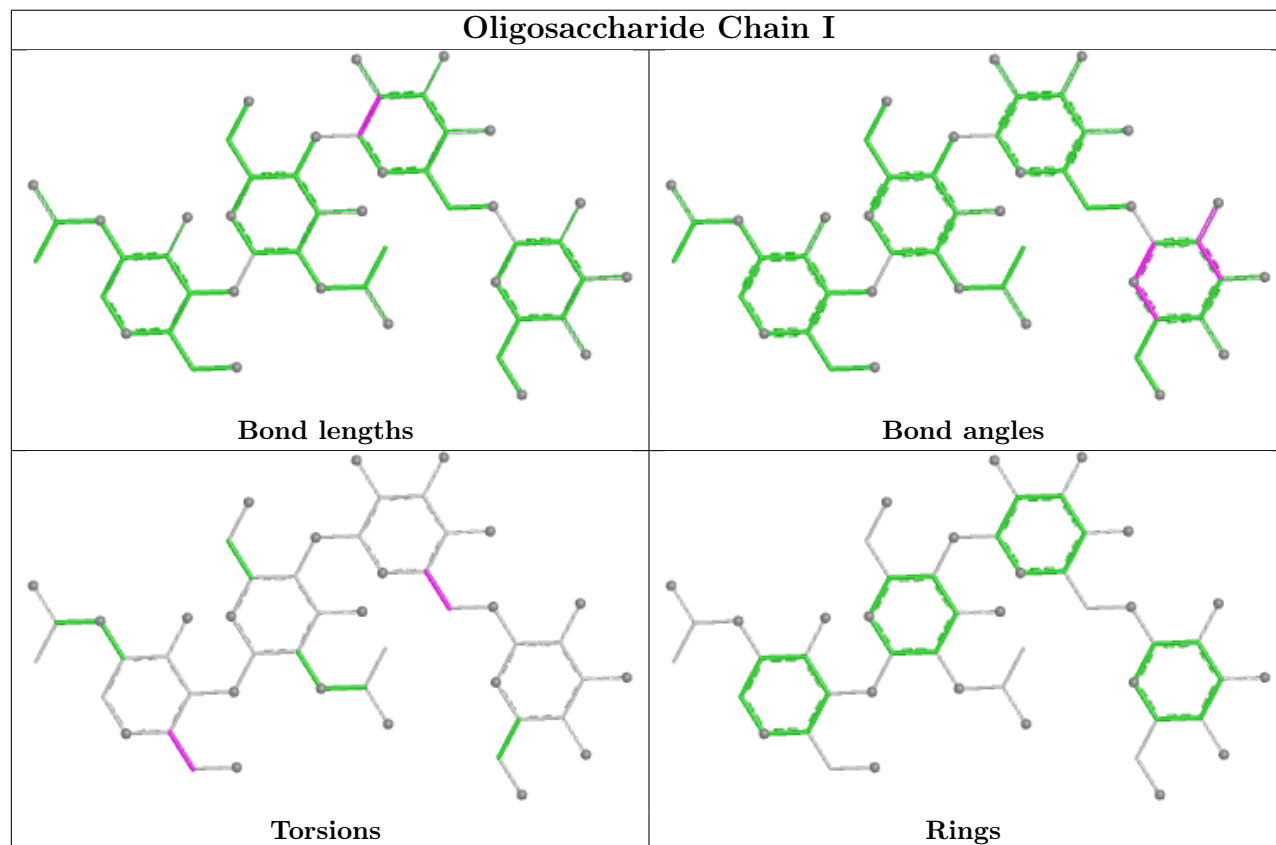
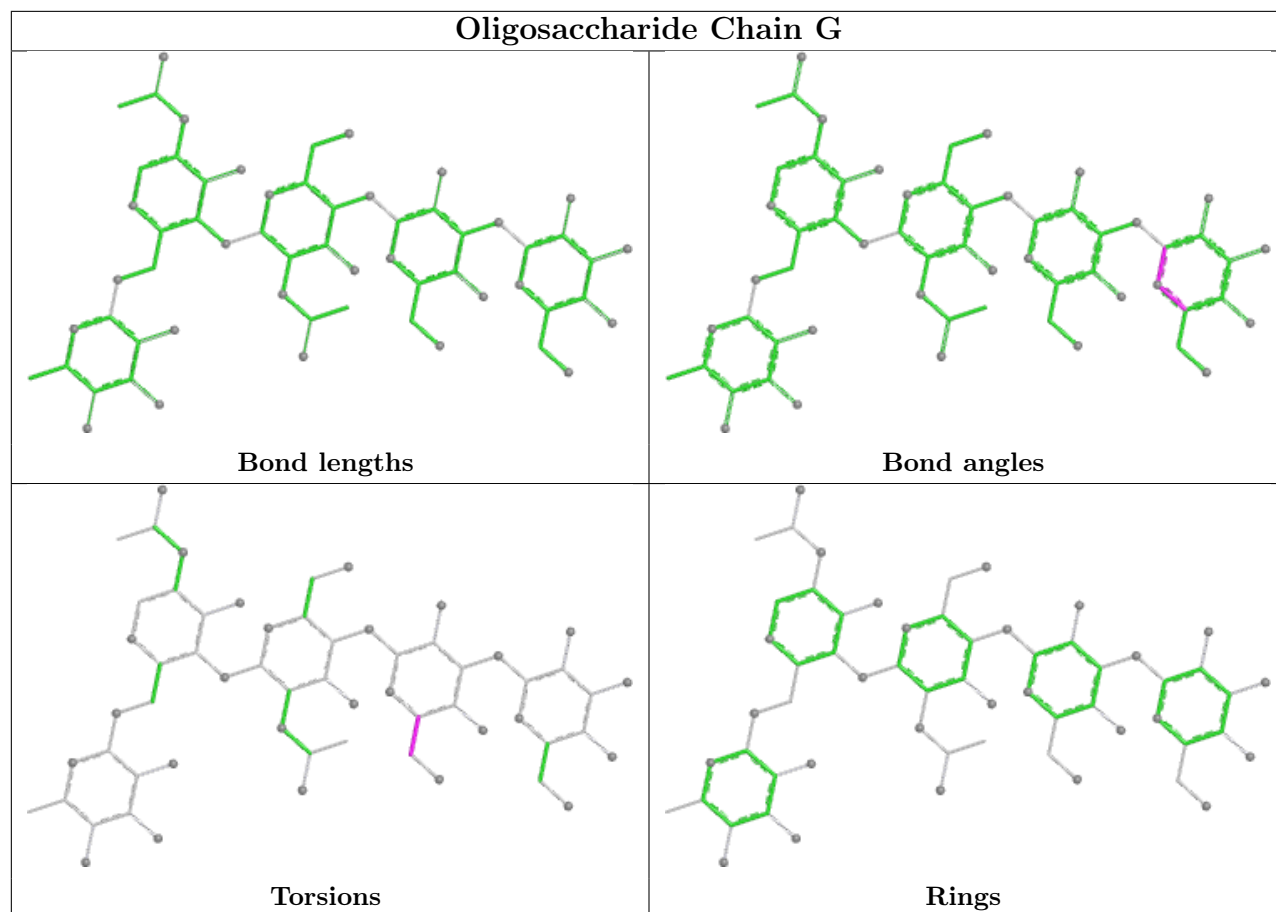


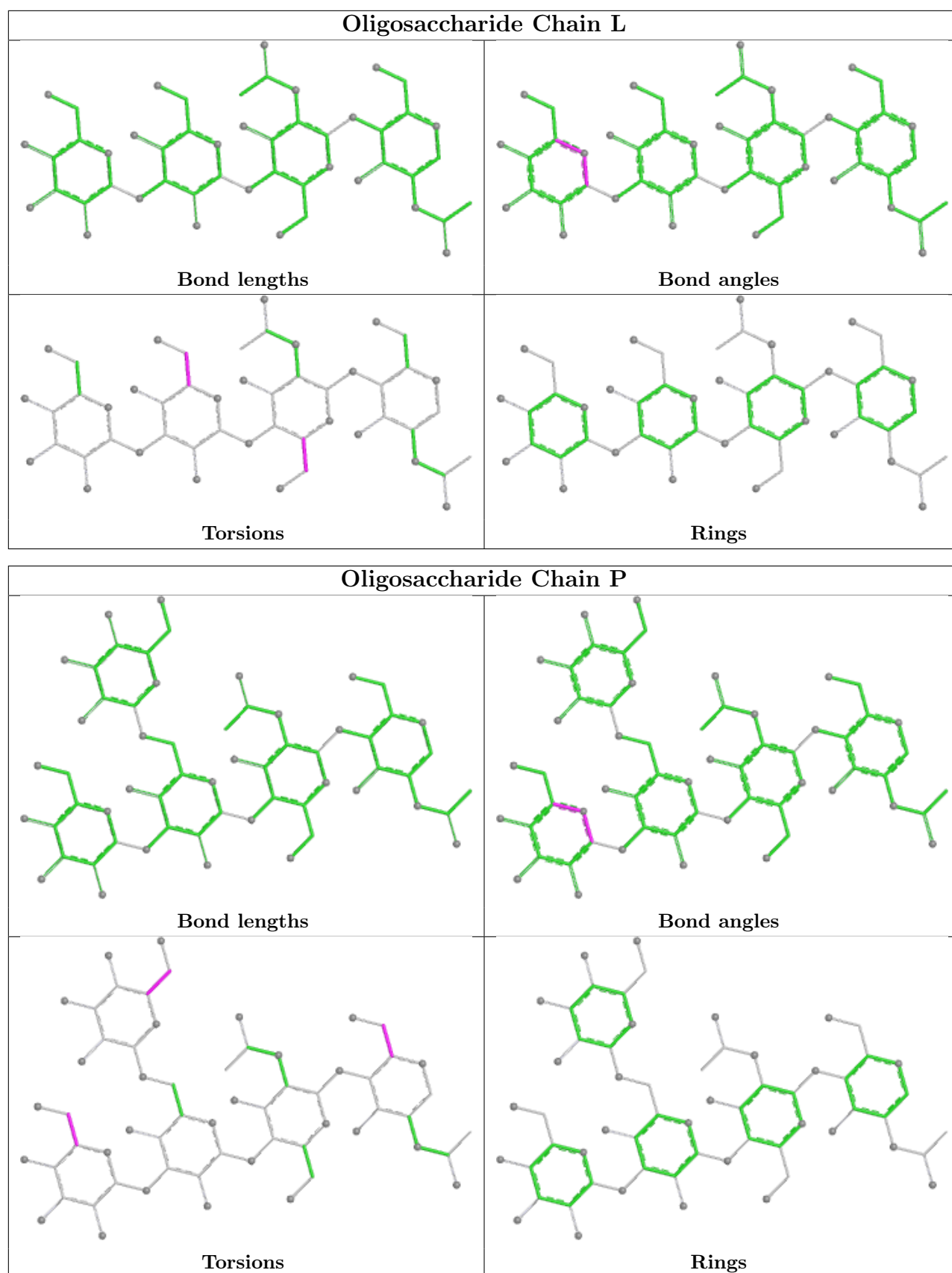












## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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
11	NAG	A	930	1	14,14,15	0.24	0	17,19,21	0.44	0
11	NAG	B	929	1	14,14,15	0.76	1 (7%)	17,19,21	1.52	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	A	930	1	-	2/6/23/26	0/1/1/1
11	NAG	B	929	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	929	NAG	O5-C1	2.67	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	929	NAG	C1-O5-C5	5.83	120.00	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	930	NAG	O5-C5-C6-O6
11	A	930	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
11	B	929	NAG	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	819/838 (97%)	-0.21	22 (2%) 56 58	22, 40, 86, 151	0
1	B	807/838 (96%)	-0.09	31 (3%) 44 46	22, 44, 96, 168	0
All	All	1626/1676 (97%)	-0.15	53 (3%) 49 51	22, 42, 90, 168	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	145	ASP	5.2
1	B	73	VAL	5.0
1	A	146	THR	4.3
1	B	62	SER	4.1
1	B	871	PHE	4.1

### 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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	E	2	14/15	0.52	0.18	87,94,111,113	0
2	NAG	R	1	14/15	0.54	0.16	62,74,86,90	0
4	NAG	O	2	14/15	0.56	0.15	95,104,124,125	0
3	BMA	F	3	11/12	0.59	0.15	77,86,100,103	0
7	MAN	L	4	11/12	0.61	0.14	91,97,115,116	0

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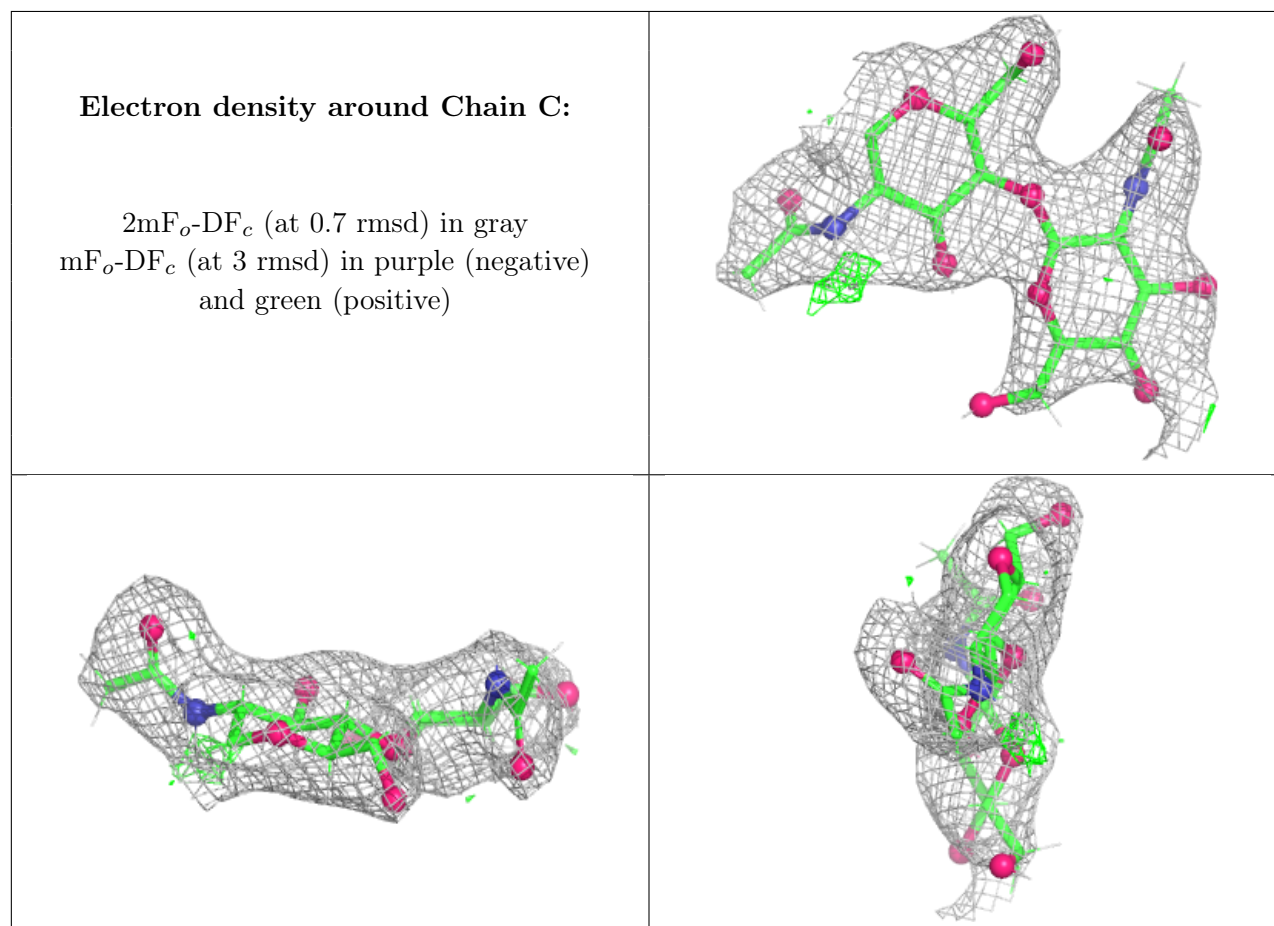
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BMA	N	3	11/12	0.62	0.13	78,83,100,100	0
3	BMA	D	3	11/12	0.62	0.13	69,75,88,90	0
2	NAG	R	2	14/15	0.63	0.17	86,92,109,111	0
5	BMA	G	3	11/12	0.64	0.13	77,82,98,98	0
4	NAG	H	2	14/15	0.65	0.15	100,108,128,129	0
4	FUC	O	3	10/11	0.66	0.17	84,87,104,105	0
4	NAG	H	1	14/15	0.67	0.15	72,88,106,106	0
4	FUC	J	3	10/11	0.67	0.20	81,90,104,108	0
4	NAG	J	2	14/15	0.68	0.19	89,97,115,116	0
4	NAG	M	2	14/15	0.68	0.14	81,85,101,102	0
4	FUC	H	3	10/11	0.70	0.17	91,94,113,113	0
7	BMA	L	3	11/12	0.74	0.10	72,80,95,96	0
5	MAN	G	4	11/12	0.76	0.18	82,86,101,102	0
2	NAG	K	2	14/15	0.77	0.15	67,81,96,101	0
4	FUC	E	3	10/11	0.77	0.17	87,90,108,109	0
4	NAG	Q	2	14/15	0.79	0.12	73,79,95,95	0
6	NAG	I	1	14/15	0.79	0.12	43,61,76,77	0
4	FUC	M	3	10/11	0.80	0.15	78,81,97,98	0
4	NAG	J	1	14/15	0.81	0.13	56,72,86,86	0
6	BMA	I	3	11/12	0.82	0.13	52,63,75,76	0
6	NAG	I	2	14/15	0.83	0.14	67,73,88,90	0
2	NAG	C	2	14/15	0.83	0.13	65,77,92,93	0
4	NAG	O	1	14/15	0.84	0.11	63,80,93,96	0
6	MAN	I	4	11/12	0.87	0.12	56,65,76,79	0
4	FUC	Q	3	10/11	0.87	0.12	69,74,85,89	0
4	NAG	E	1	14/15	0.87	0.10	50,66,84,87	0
5	NAG	G	2	14/15	0.88	0.10	59,68,79,82	0
4	NAG	M	1	14/15	0.88	0.10	51,68,80,82	0
3	NAG	N	2	14/15	0.88	0.11	41,55,71,72	0
8	MAN	P	5	11/12	0.88	0.11	52,57,69,69	0
2	NAG	K	1	14/15	0.90	0.10	39,51,61,68	0
8	NAG	P	1	14/15	0.90	0.09	38,47,55,57	0
8	NAG	P	2	14/15	0.90	0.10	48,56,69,69	0
8	MAN	P	4	11/12	0.90	0.11	52,59,69,71	0
3	NAG	F	2	14/15	0.90	0.10	43,54,66,71	0
3	NAG	D	2	14/15	0.91	0.09	47,57,68,71	0
7	NAG	L	2	14/15	0.91	0.09	46,56,67,71	0
2	NAG	C	1	14/15	0.91	0.09	41,52,62,65	0
5	FUC	G	5	10/11	0.91	0.09	44,48,57,58	0
4	NAG	Q	1	14/15	0.92	0.07	52,64,75,77	0
5	NAG	G	1	14/15	0.93	0.08	36,47,54,57	0
8	BMA	P	3	11/12	0.94	0.08	45,50,59,61	0

*Continued on next page...*

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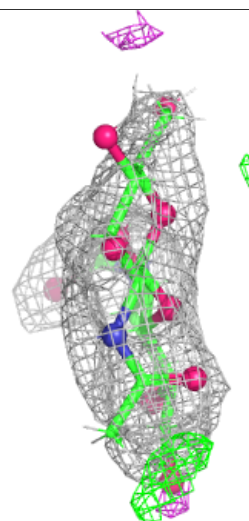
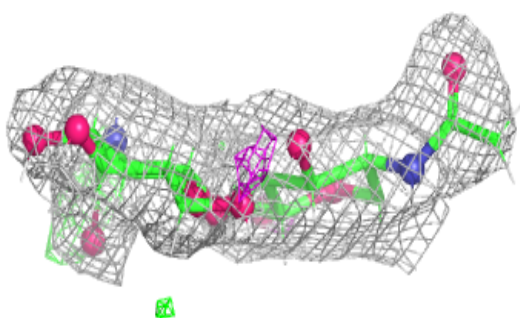
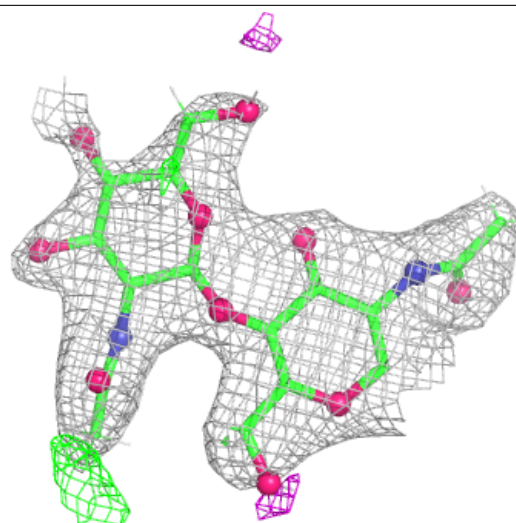
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	L	1	14/15	0.94	0.08	25,39,47,52	0
3	NAG	D	1	14/15	0.94	0.07	28,42,52,53	0
3	NAG	F	1	14/15	0.97	0.05	22,29,36,36	0
3	NAG	N	1	14/15	0.98	0.04	18,27,32,35	0

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.



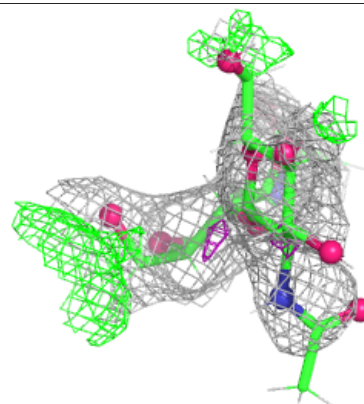
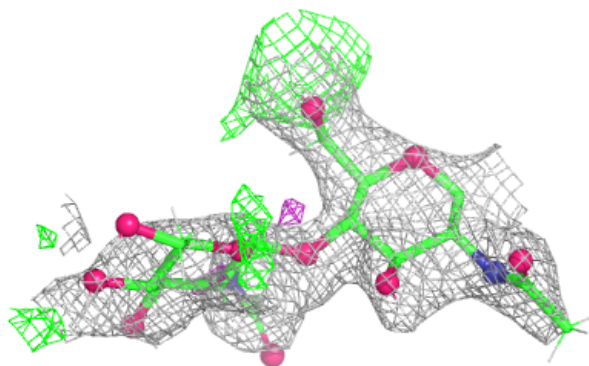
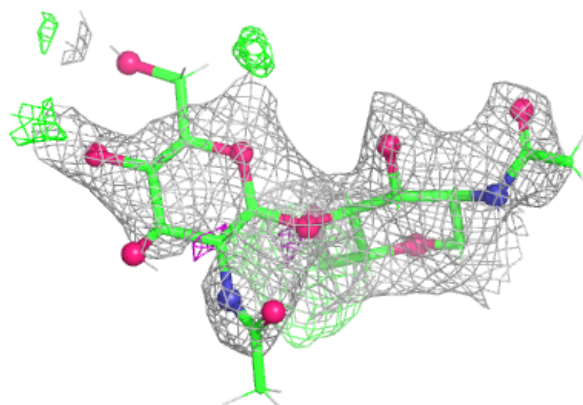
**Electron density around Chain K:**

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

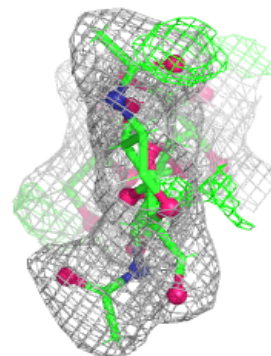
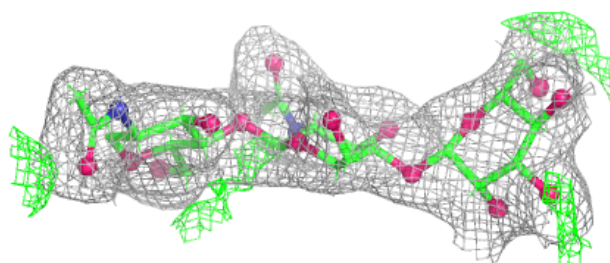
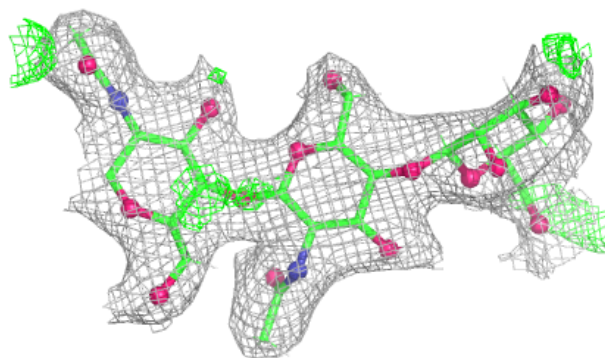


**Electron density around Chain R:**

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

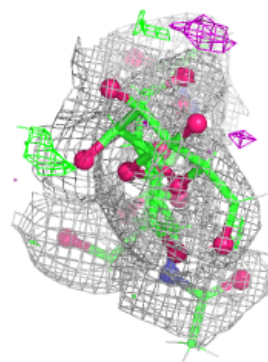
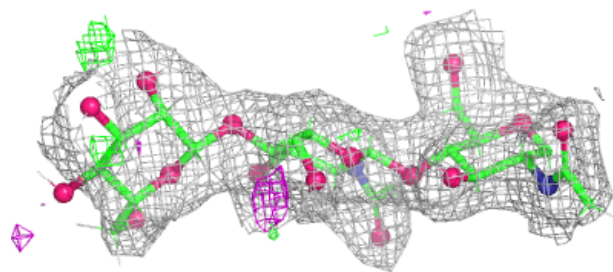
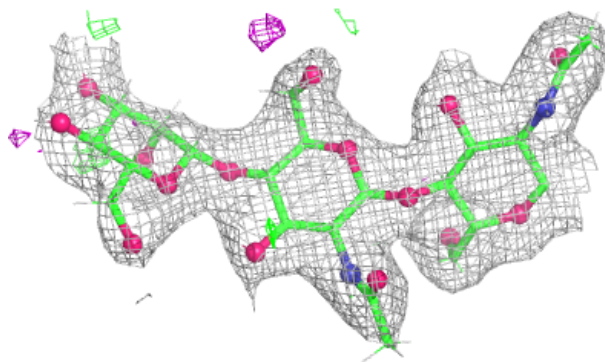
**Electron density around Chain D:**

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

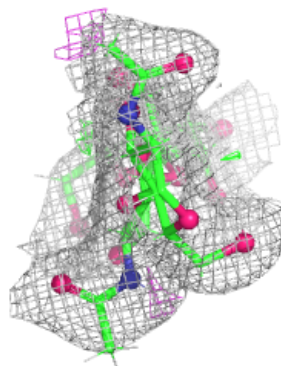
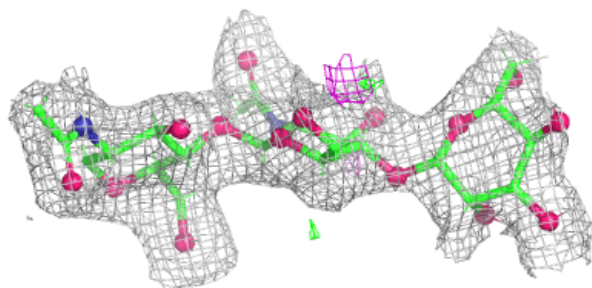
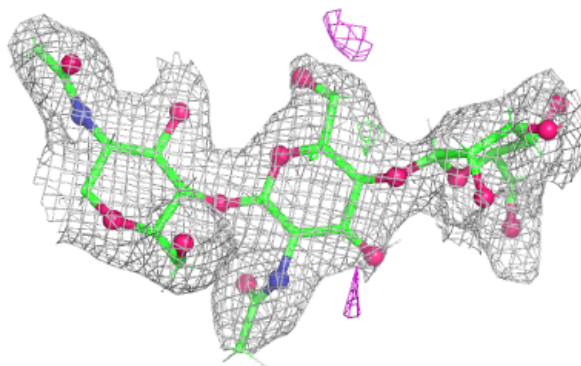


**Electron density around Chain F:**

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

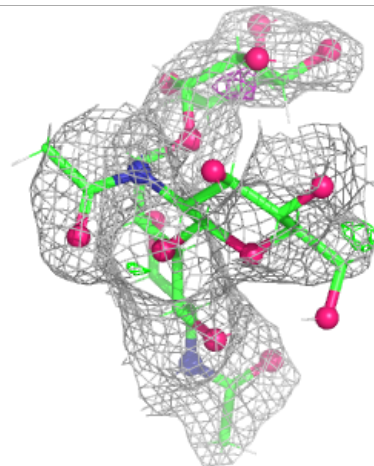
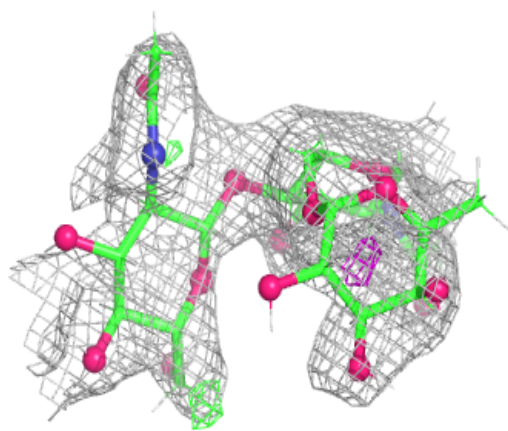
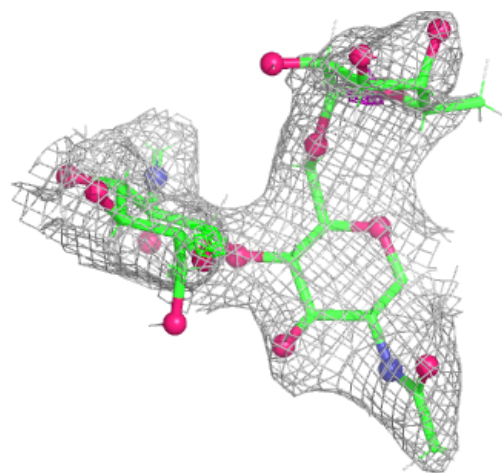
**Electron density around Chain N:**

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



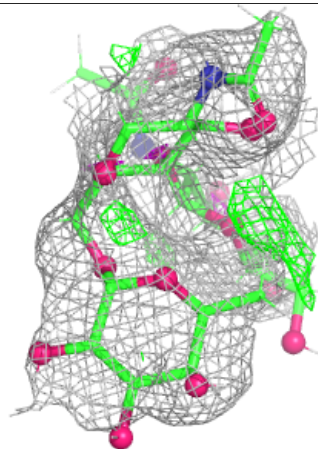
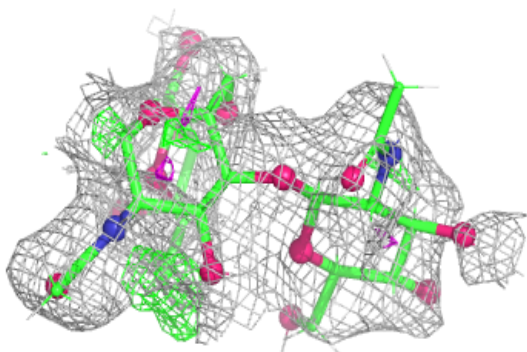
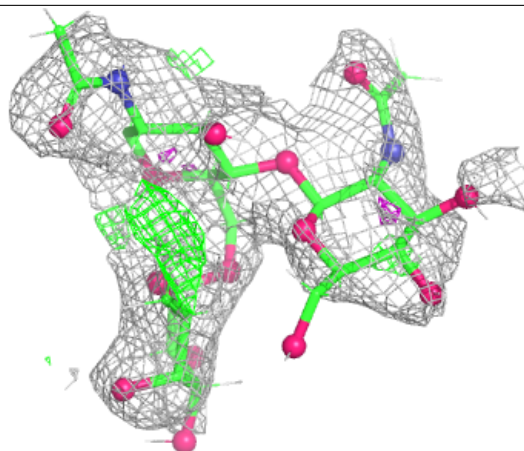
**Electron density around Chain E:**

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



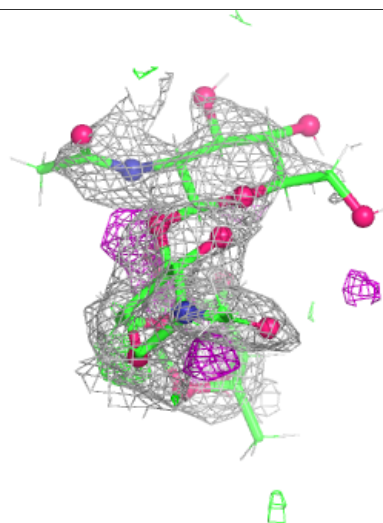
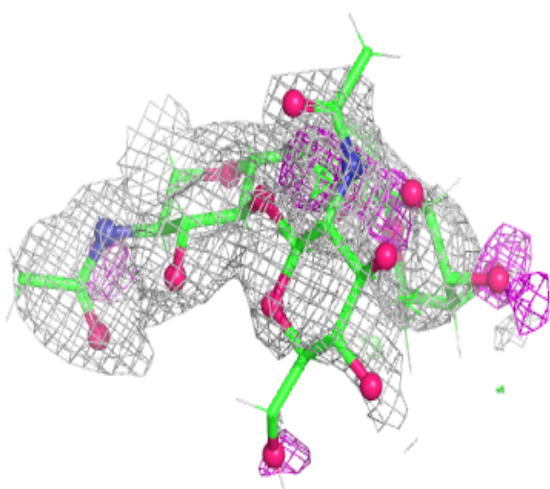
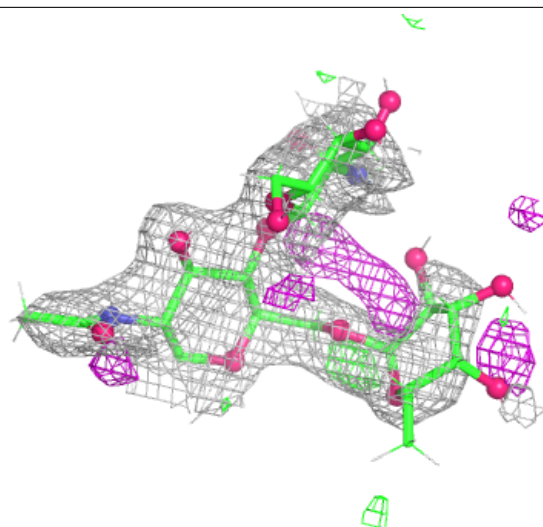
**Electron density around Chain H:**

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



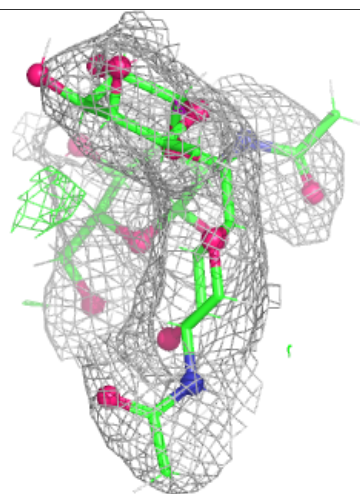
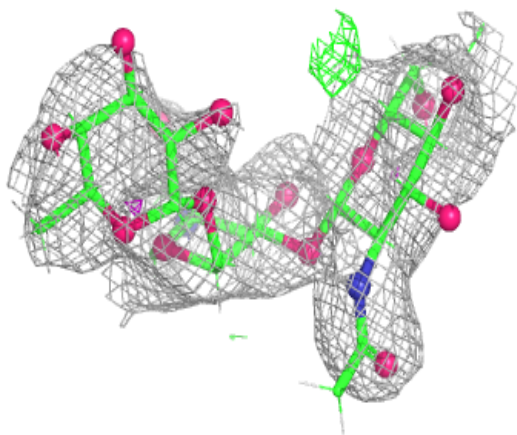
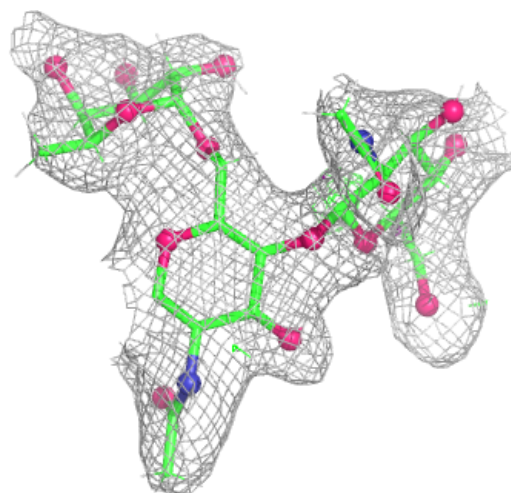
**Electron density around Chain J:**

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



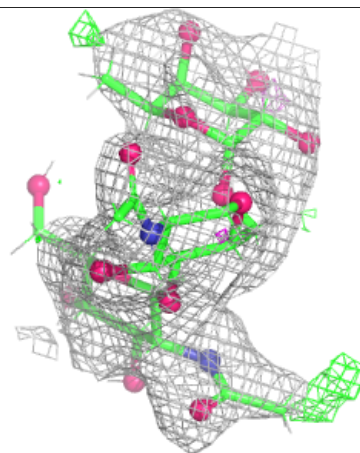
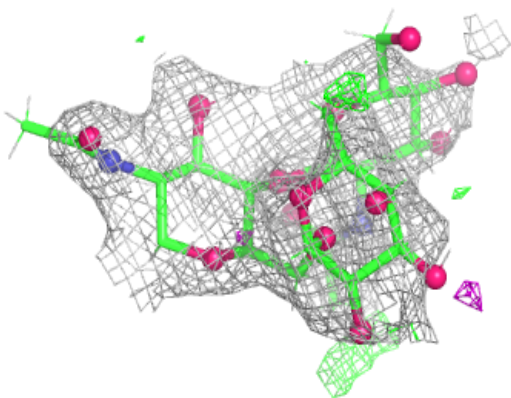
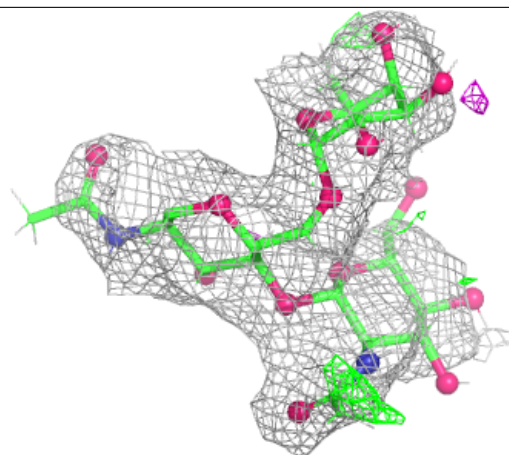
**Electron density around Chain M:**

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



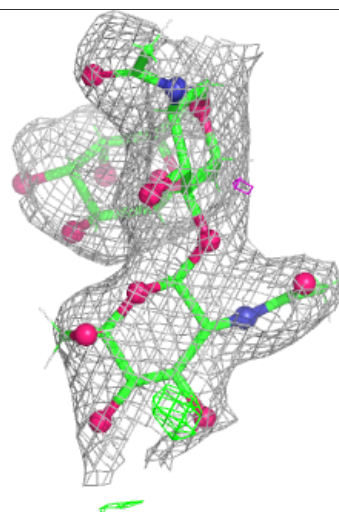
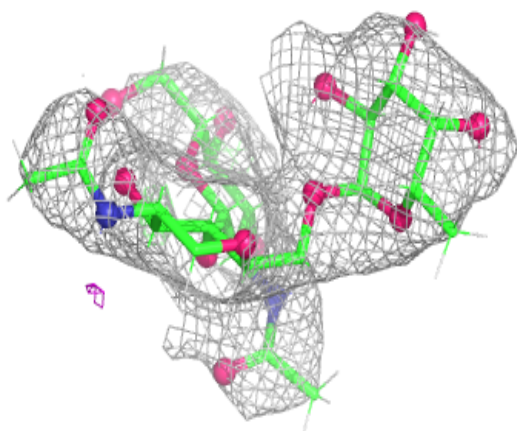
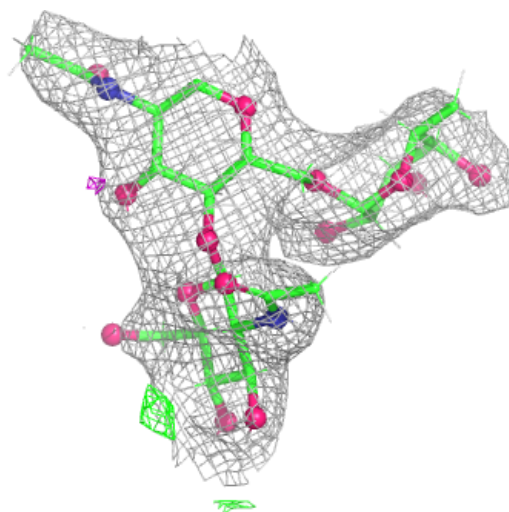
**Electron density around Chain O:**

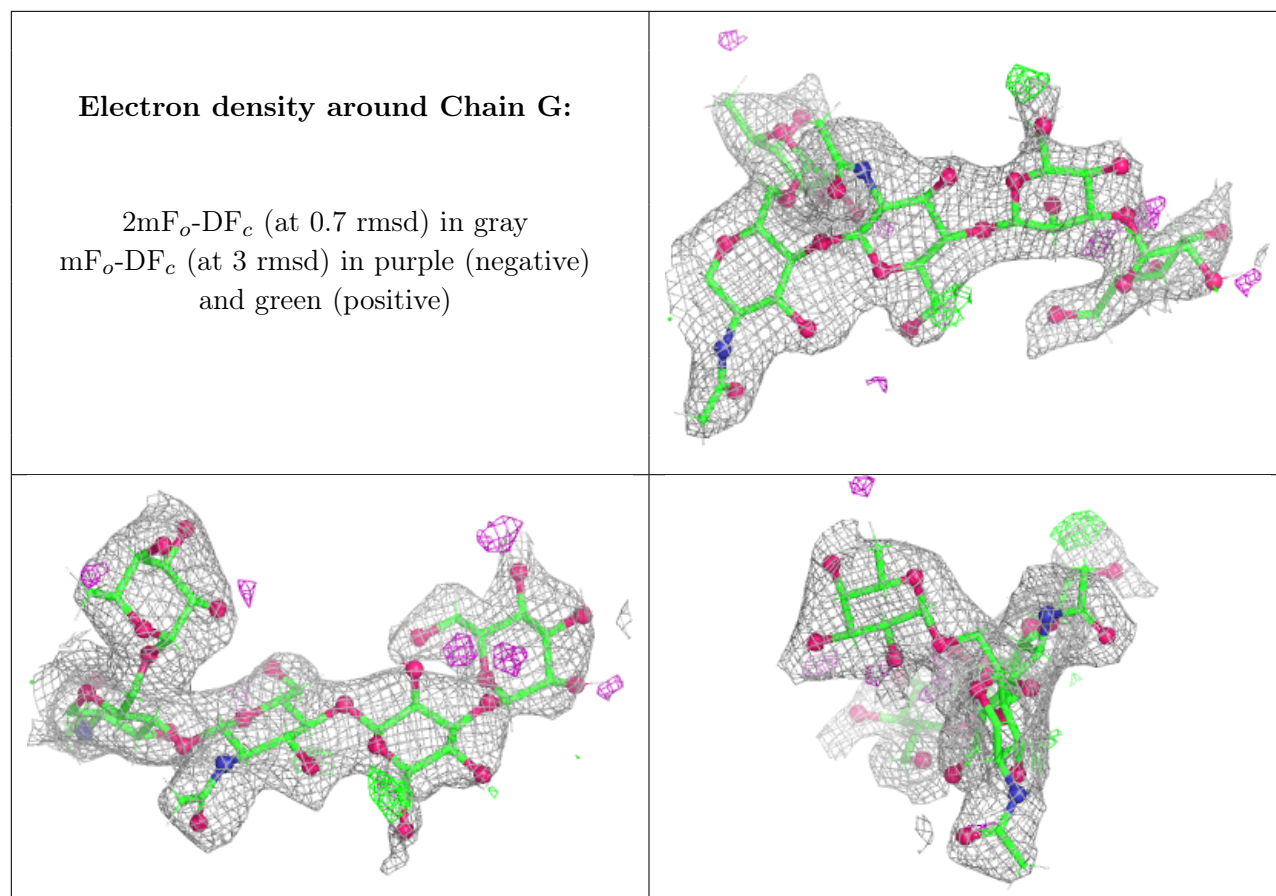
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain Q:**

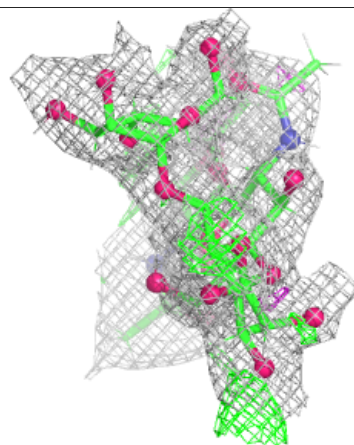
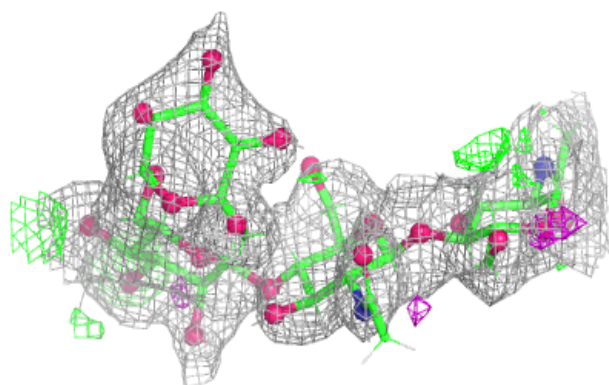
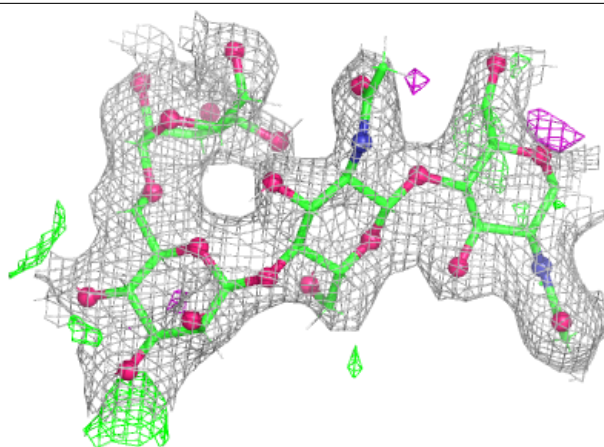
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



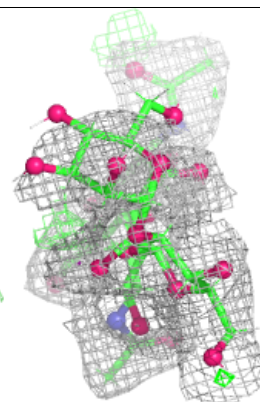
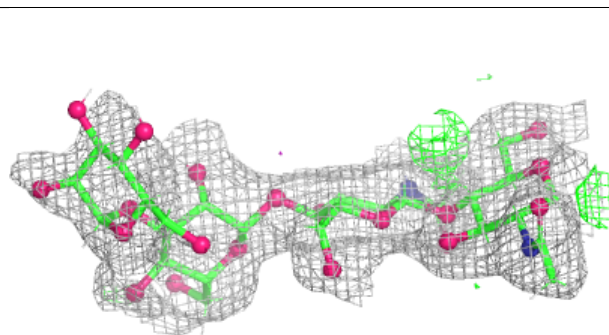
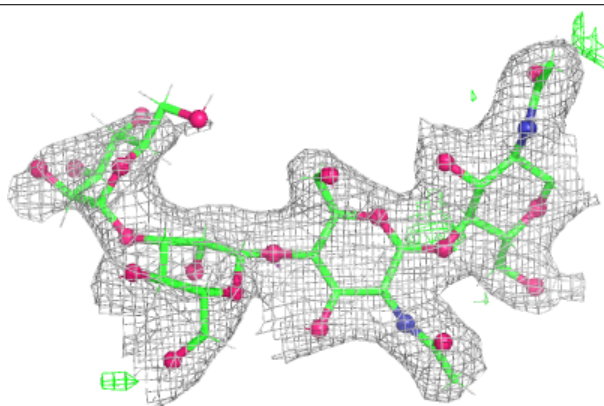


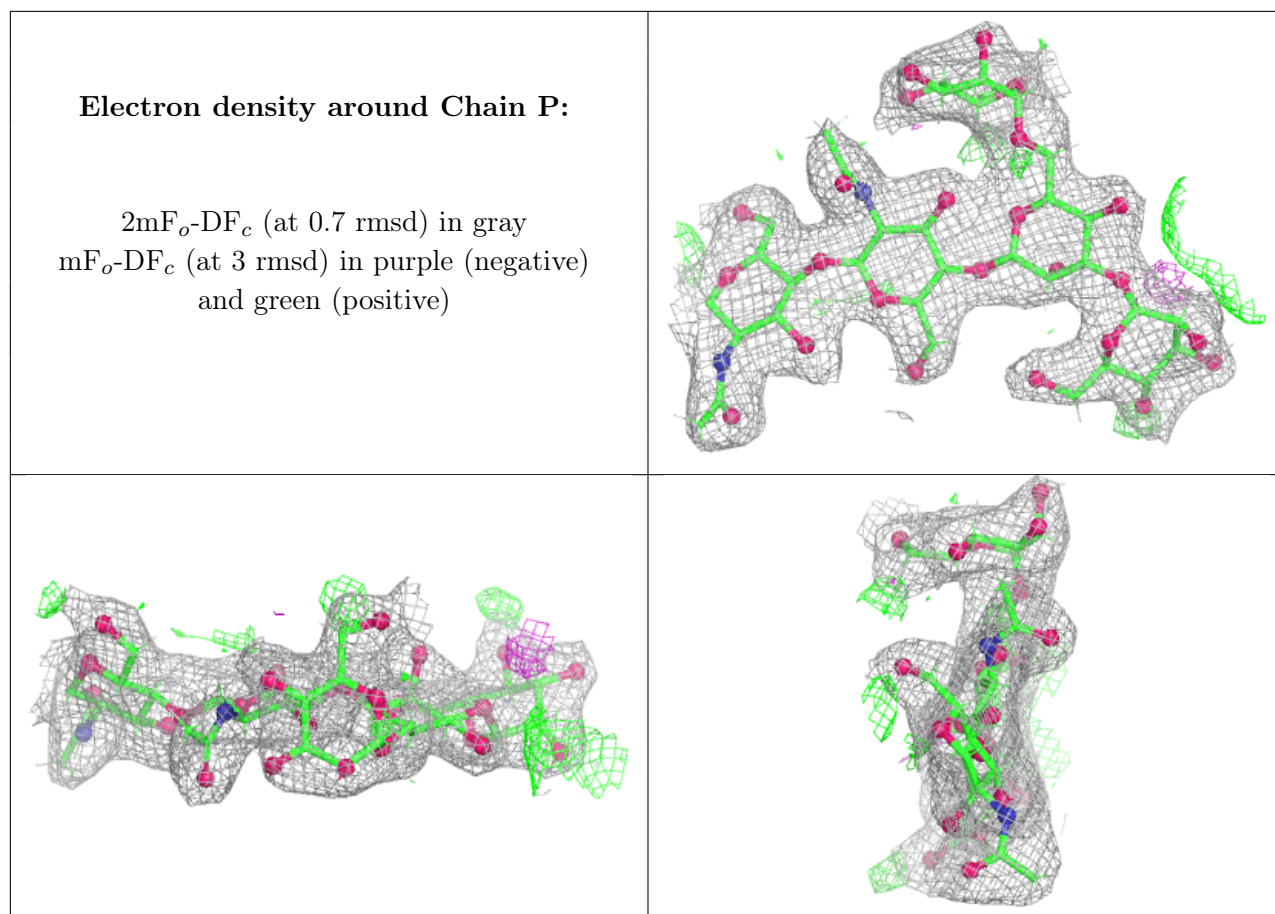
**Electron density around Chain I:**

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

**Electron density around Chain L:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
11	NAG	B	929	14/15	0.55	0.18	74,85,101,102	0
11	NAG	A	930	14/15	0.67	0.17	72,85,101,102	0
12	NA	B	930	1/1	0.93	0.07	56,56,56,56	0
12	NA	A	931	1/1	0.96	0.07	58,58,58,58	0
9	ZN	A	901	1/1	0.98	0.06	28,28,28,28	0
9	ZN	B	901	1/1	0.99	0.03	29,29,29,29	0
9	ZN	B	902	1/1	0.99	0.03	33,33,33,33	0
9	ZN	A	902	1/1	0.99	0.04	34,34,34,34	0
10	CA	A	903	1/1	1.00	0.01	28,28,28,28	0
10	CA	B	903	1/1	1.00	0.01	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.