



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 26, 2023 – 02:22 PM EDT

PDB ID : 6C02
Title : Human ectonucleotide pyrophosphatase / phosphodiesterase 3 (ENPP3, NPP3, CD203c), inactive (T205A), N594S, with alpha,beta-methylene-A TP (AMPCPP)
Authors : Gorelik, A.; Randriamihaja, A.; Illes, K.; Nagar, B.
Deposited on : 2017-12-27
Resolution : 1.94 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

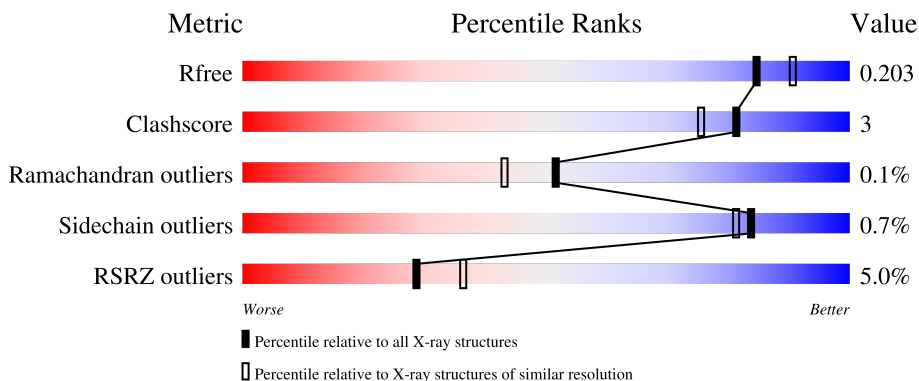
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 Å.

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





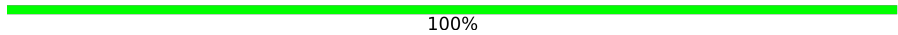


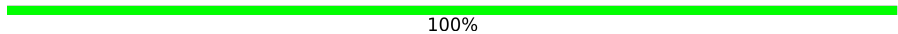
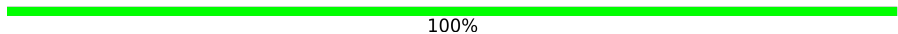
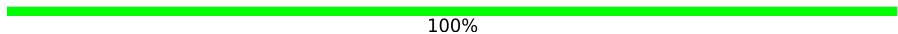
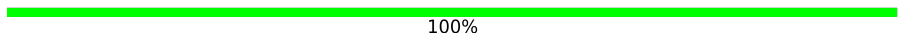

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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

Mol	Chain	Length	Quality of chain
1	A	838	 3% (Poor fit), 91% (0-3 outliers), 6% (4+ outliers)
1	B	838	 6% (Poor fit), 90% (0-3 outliers), 7% (4+ outliers)
2	C	2	 100%
2	F	2	 100%

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Mol	Chain	Length	Quality of chain
2	J	2	 50% 50%
2	L	2	 50% 50%
2	M	2	 100%
3	D	3	 67% 33%
3	K	3	 67% 33%
4	E	3	 100%
4	G	3	 100%
4	N	3	 100%
5	H	2	 100%
5	I	2	 50% 50%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 27835 atoms, of which 12913 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	815	12832	4182	6260	1118	1215	57	0	0	0
1	B	815	12833	4182	6261	1118	1215	57	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

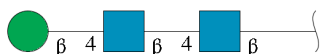
Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ASP	-	expression tag	UNP O14638
A	39	ARG	-	expression tag	UNP O14638
A	40	HIS	-	expression tag	UNP O14638
A	41	HIS	-	expression tag	UNP O14638
A	42	HIS	-	expression tag	UNP O14638
A	43	HIS	-	expression tag	UNP O14638
A	44	HIS	-	expression tag	UNP O14638
A	45	HIS	-	expression tag	UNP O14638
A	46	LYS	-	expression tag	UNP O14638
A	47	LEU	-	expression tag	UNP O14638
A	205	ALA	THR	engineered mutation	UNP O14638
A	594	SER	ASN	engineered mutation	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
B	205	ALA	THR	engineered mutation	UNP O14638
B	594	SER	ASN	engineered mutation	UNP O14638

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



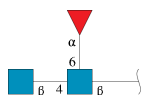
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	F	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	J	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	L	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	M	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- 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	K	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	G	3	Total	C	H	N	O	0	0	0
			74	22	36	2	14			

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

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	2	Total	C	H	N	O	0	0	0
			47	14	23	1	9			
5	I	2	Total	C	H	N	O	0	0	0
			47	14	23	1	9			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

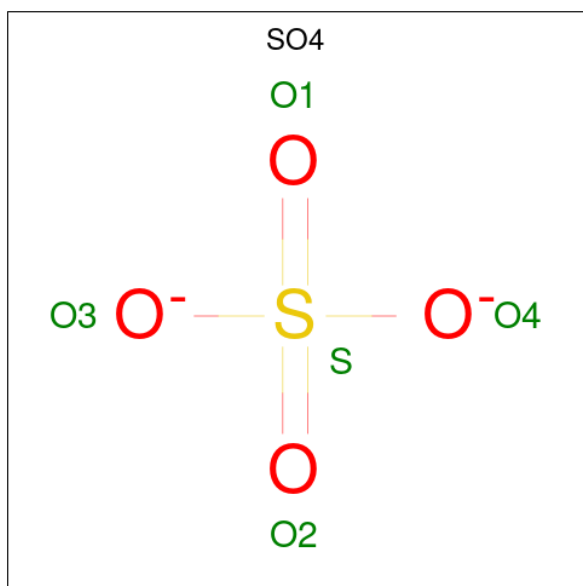
- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

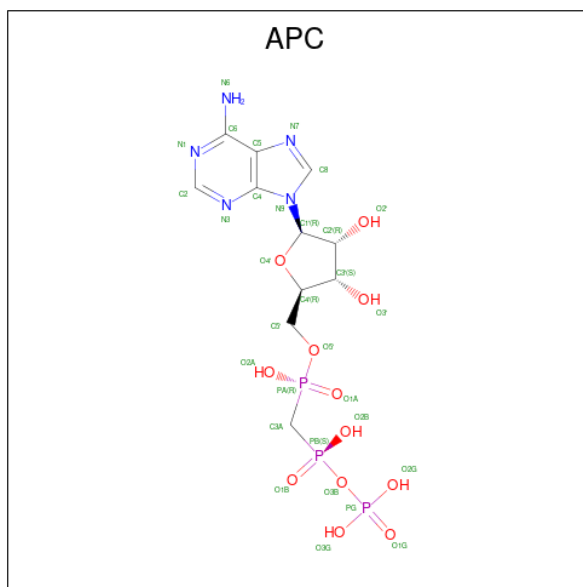
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total	Cl	0	0
			3	3		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
11	A	1	44	11	13	5	12	3	0	0
11	B	1	45	11	14	5	12	3	0	0

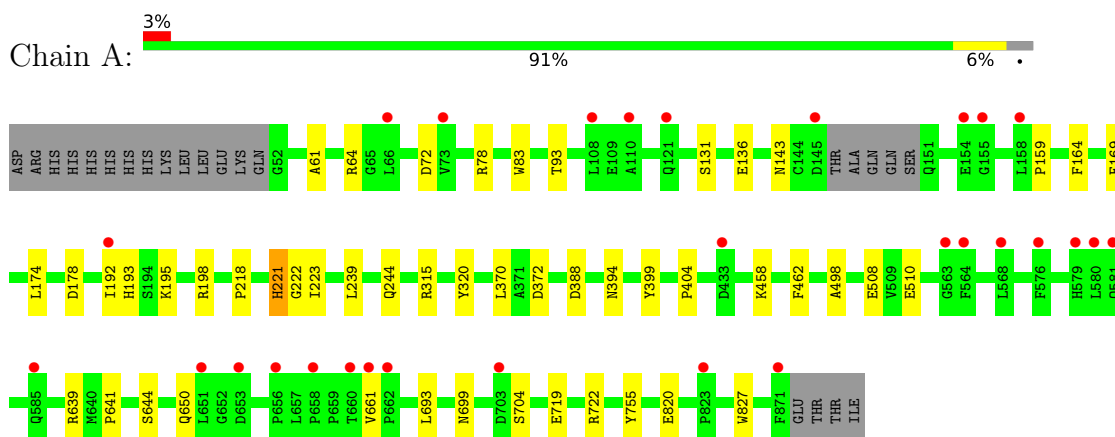
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	685	685	685	0	0
12	B	620	620	620	0	0

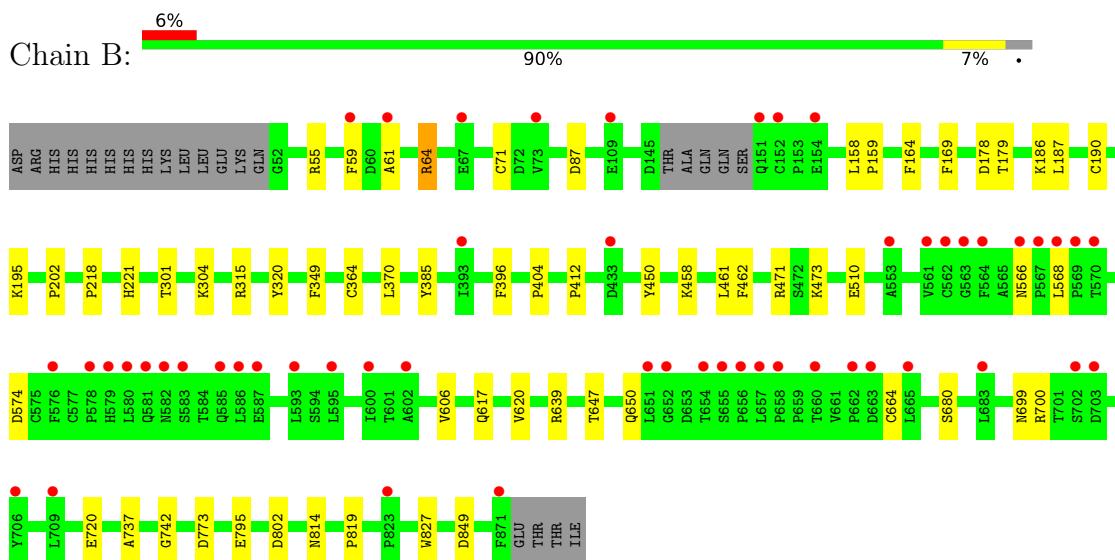
3 Residue-property plots [i](#)

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

- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3



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



MAG1
MAG2

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

Chain F:  100%MAG1
MAG2

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

Chain J:  50% 50%MAG1
MAG2

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

Chain L:  50% 50%MAG1
MAG2

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

Chain M:  100%MAG1
MAG2

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

Chain D:  67% 33%MAG1
MAG2
EMAS

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

Chain K:  67% 33%MAG1
MAG2
EMAS

- 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 G:  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 N:  100%

MAG1
MAG2
FUC3

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1
FUC2

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

MAG1
FUC2

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.66Å 169.46Å 79.06Å 90.00° 103.87° 90.00°	Depositor
Resolution (Å)	48.62 – 1.94 48.62 – 1.94	Depositor EDS
% Data completeness (in resolution range)	84.2 (48.62-1.94) 80.0 (48.62-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 1.94Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.166 , 0.197 0.172 , 0.203	Depositor DCC
R_{free} test set	1987 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.247 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27835	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAG, FUC, ZN, CL, CA, BMA, NA, APC

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	0.30	0/6769	0.47	0/9202
1	B	0.29	0/6769	0.47	0/9202
All	All	0.30	0/13538	0.47	0/18404

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6572	6260	6259	35	1
1	B	6572	6261	6261	34	1
2	C	28	27	25	0	0
2	F	28	27	25	0	0
2	J	28	27	25	0	0
2	L	28	27	25	0	0
2	M	28	27	25	0	0
3	D	39	37	34	0	0
3	K	39	37	34	0	0
4	E	38	37	34	0	0
4	G	38	36	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	38	37	34	0	0
5	H	24	23	22	0	0
5	I	24	23	22	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	3	0	0	0	0
10	A	10	0	0	0	0
10	B	10	0	0	0	0
11	A	31	13	13	3	0
11	B	31	14	13	2	0
12	A	685	0	0	9	2
12	B	620	0	0	10	2
All	All	14922	12913	12885	69	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 69 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:699:ASN:O	12:B:1001:HOH:O	2.00	0.80
1:A:820:GLU:OE1	12:A:1001:HOH:O	2.04	0.75
1:B:720:GLU:OE2	12:B:1002:HOH:O	2.04	0.74
1:A:61:ALA:O	1:A:64:ARG:NH1	2.19	0.74
1:A:218:PRO:HA	1:A:221:HIS:CE1	2.24	0.72

All (3) 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:143:ASN:HD21	1:B:795:GLU:OE2[1_554]	1.52	0.08
12:A:1162:HOH:O	12:B:1386:HOH:O[2_555]	2.17	0.03
12:A:1616:HOH:O	12:B:1440:HOH:O[2_555]	2.18	0.02

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	811/838 (97%)	782 (96%)	28 (4%)	1 (0%)	51	43
1	B	811/838 (97%)	779 (96%)	31 (4%)	1 (0%)	51	43
All	All	1622/1676 (97%)	1561 (96%)	59 (4%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	827	TRP
1	B	827	TRP

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	735/757 (97%)	730 (99%)	5 (1%)	84	81
1	B	735/757 (97%)	730 (99%)	5 (1%)	84	81
All	All	1470/1514 (97%)	1460 (99%)	10 (1%)	84	81

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	169	PHE
1	B	370	LEU
1	B	462	PHE
1	A	370	LEU

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Mol	Chain	Res	Type
1	A	462	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	588	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](#)

29 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	2,1	14,14,15	0.50	0	17,19,21	0.58	0
2	NAG	C	2	2	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	D	1	3,1	14,14,15	0.37	0	17,19,21	0.64	0
3	NAG	D	2	3	14,14,15	0.36	0	17,19,21	0.45	0
3	BMA	D	3	3	11,11,12	0.76	0	15,15,17	0.89	1 (6%)
4	NAG	E	1	4,1	14,14,15	0.39	0	17,19,21	0.49	0
4	NAG	E	2	4	14,14,15	0.22	0	17,19,21	0.47	0
4	FUC	E	3	4	10,10,11	0.94	0	14,14,16	0.89	0
2	NAG	F	1	2,1	14,14,15	0.29	0	17,19,21	0.77	0
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	0.60	0
4	NAG	G	1	4,1	14,14,15	0.45	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	2	4	14,14,15	0.23	0	17,19,21	0.52	0
4	FUC	G	3	4	10,10,11	0.78	0	14,14,16	0.73	0
5	NAG	H	1	5,1	14,14,15	0.42	0	17,19,21	0.51	0
5	FUC	H	2	5	10,10,11	0.75	0	14,14,16	0.70	0
5	NAG	I	1	5,1	14,14,15	0.67	1 (7%)	17,19,21	0.58	0
5	FUC	I	2	5	10,10,11	0.69	0	14,14,16	0.79	0
2	NAG	J	1	2,1	14,14,15	0.34	0	17,19,21	0.53	0
2	NAG	J	2	2	14,14,15	0.18	0	17,19,21	0.67	1 (5%)
3	NAG	K	1	3,1	14,14,15	0.34	0	17,19,21	0.57	0
3	NAG	K	2	3	14,14,15	0.30	0	17,19,21	0.42	0
3	BMA	K	3	3	11,11,12	0.81	0	15,15,17	0.90	1 (6%)
2	NAG	L	1	2,1	14,14,15	0.27	0	17,19,21	0.60	1 (5%)
2	NAG	L	2	2	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	M	1	2,1	14,14,15	0.42	0	17,19,21	0.67	0
2	NAG	M	2	2	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	N	1	4,1	14,14,15	0.44	0	17,19,21	0.60	0
4	NAG	N	2	4	14,14,15	0.24	0	17,19,21	0.47	0
4	FUC	N	3	4	10,10,11	0.64	0	14,14,16	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUC	I	2	5	-	-	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	FUC	N	3	4	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1	NAG	C1-C2	2.26	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	O2-C2-C3	-2.42	105.29	110.14
3	K	3	BMA	C1-O5-C5	2.32	115.33	112.19
2	J	2	NAG	C1-O5-C5	2.30	115.31	112.19
2	L	1	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

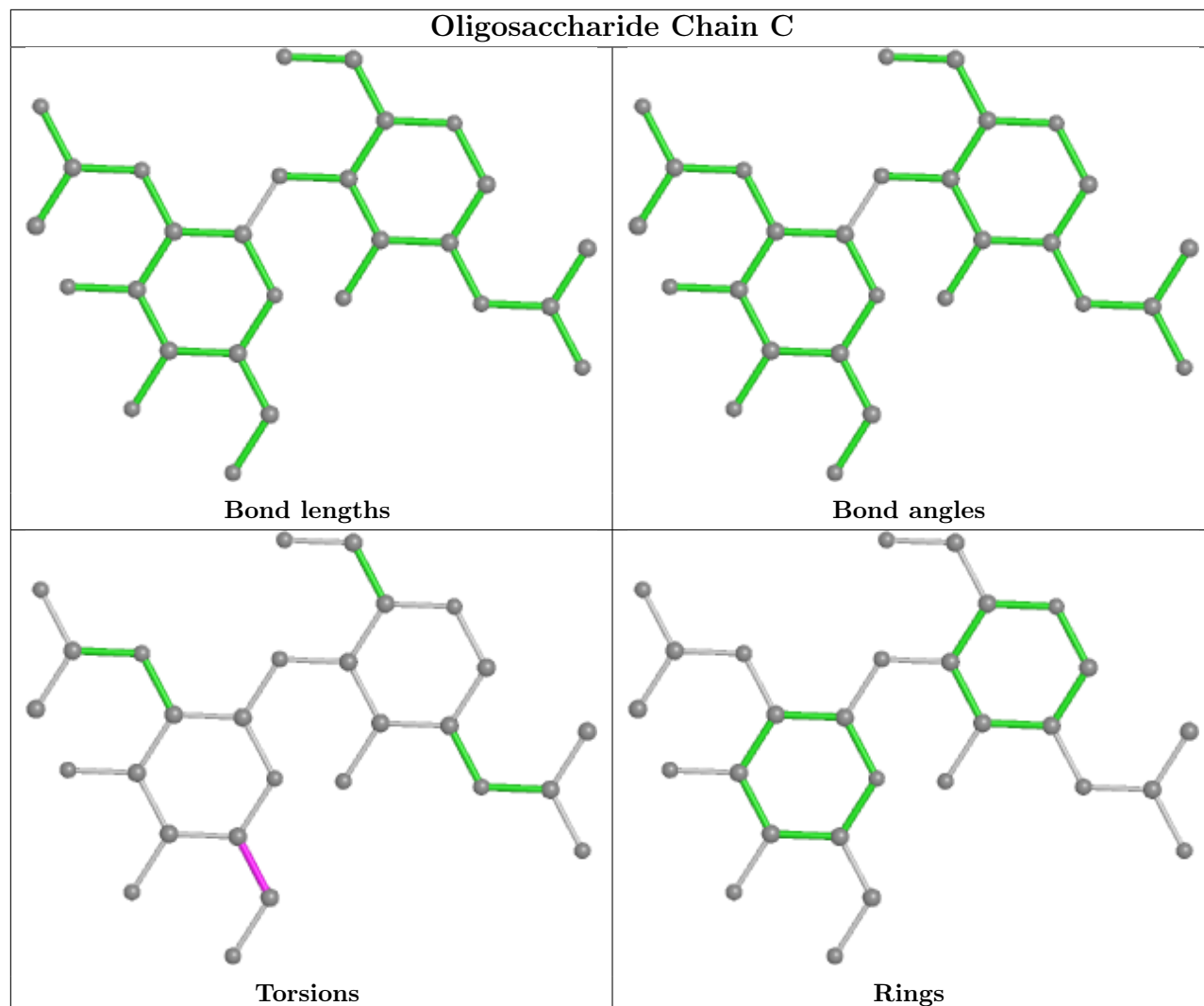
Mol	Chain	Res	Type	Atoms
2	L	2	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6

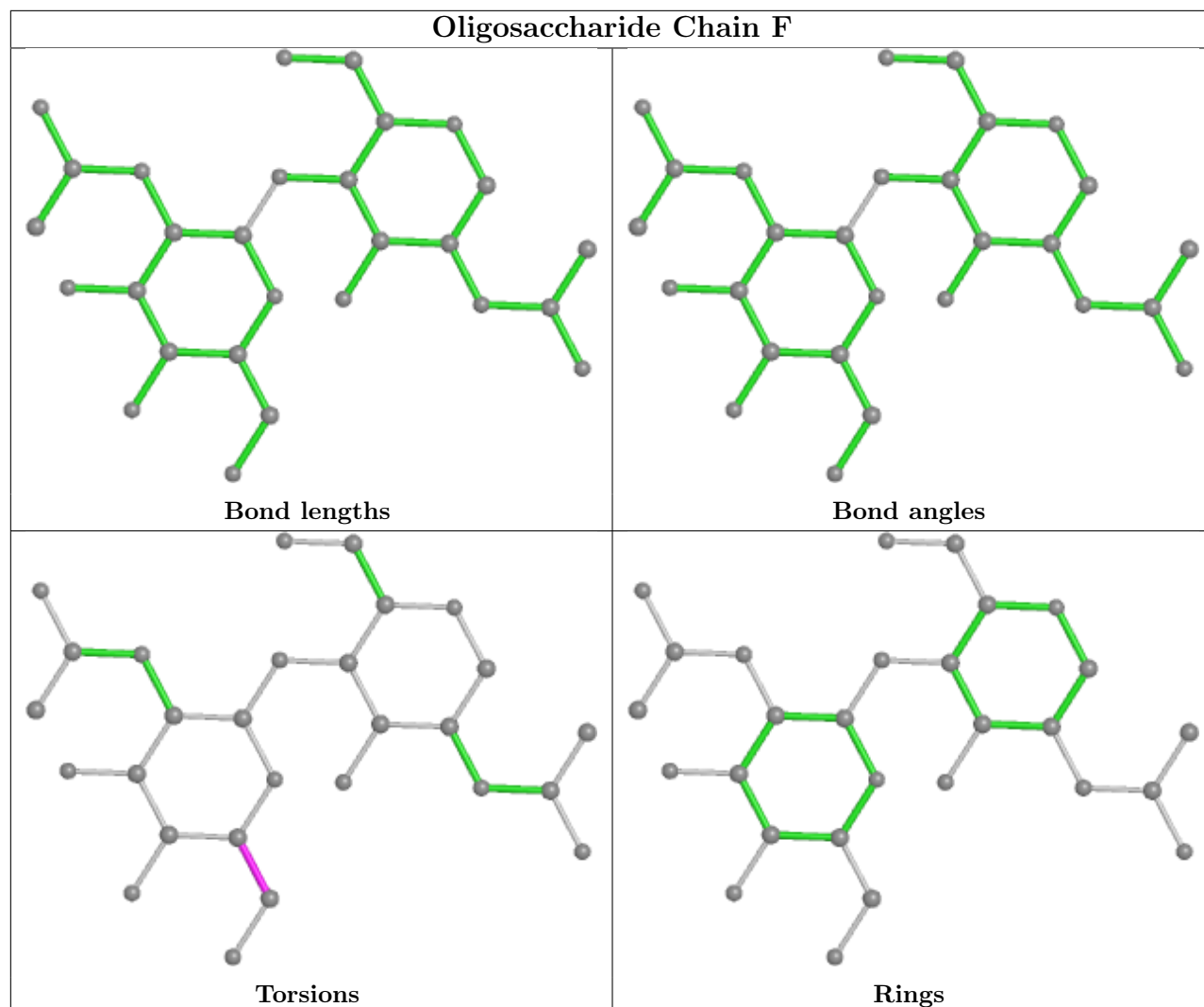
There are no ring outliers.

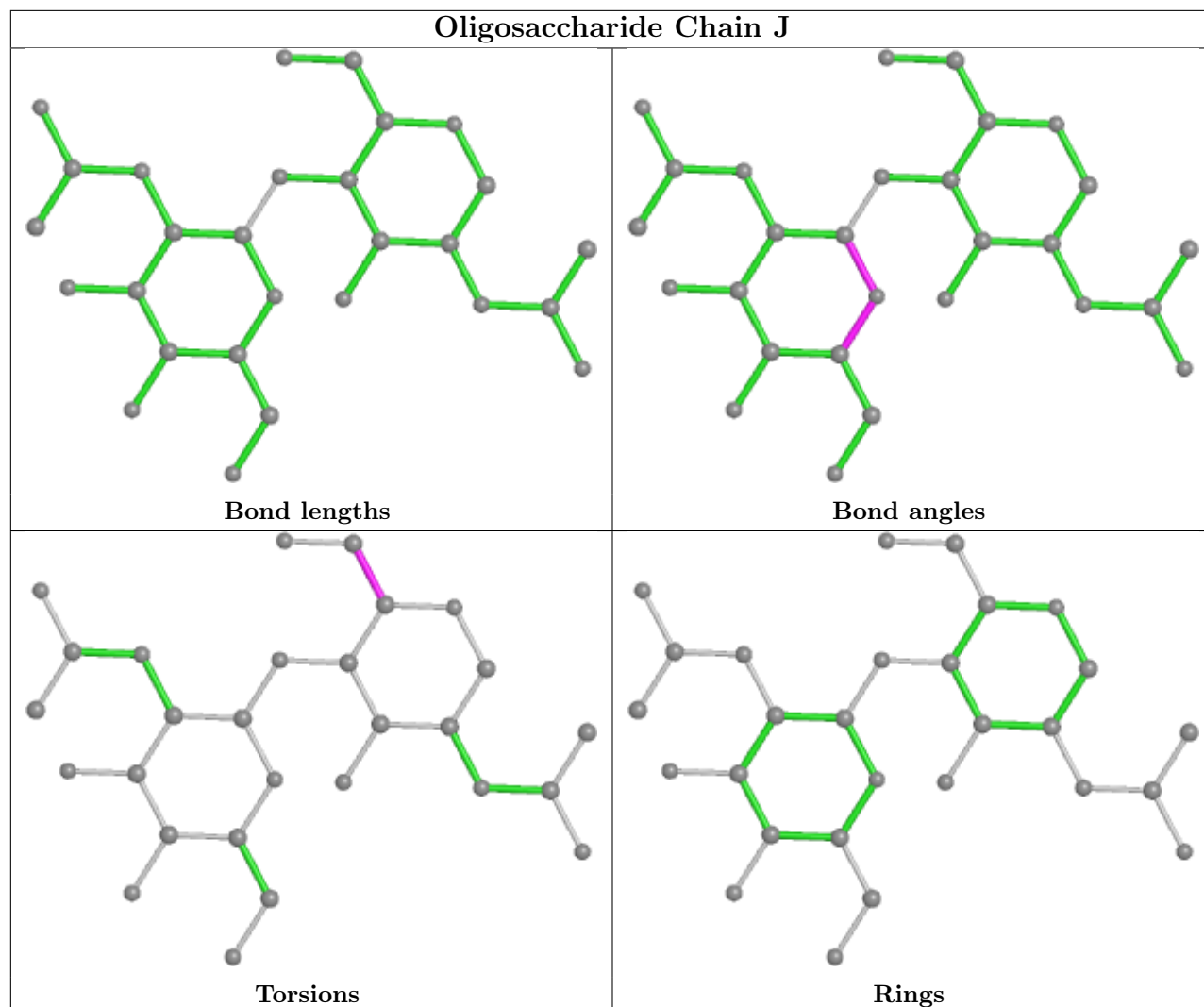
No monomer is involved in short contacts.

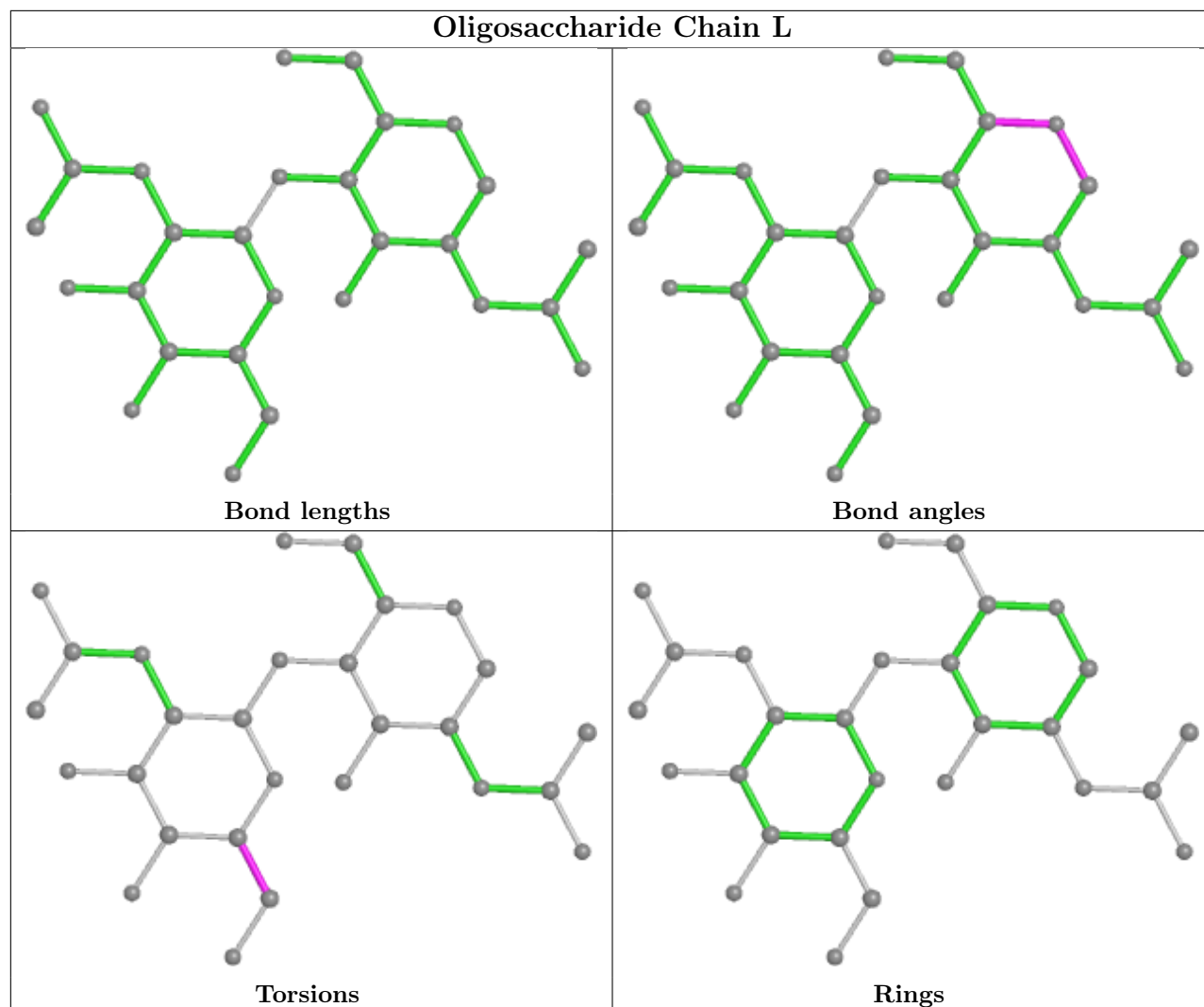
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

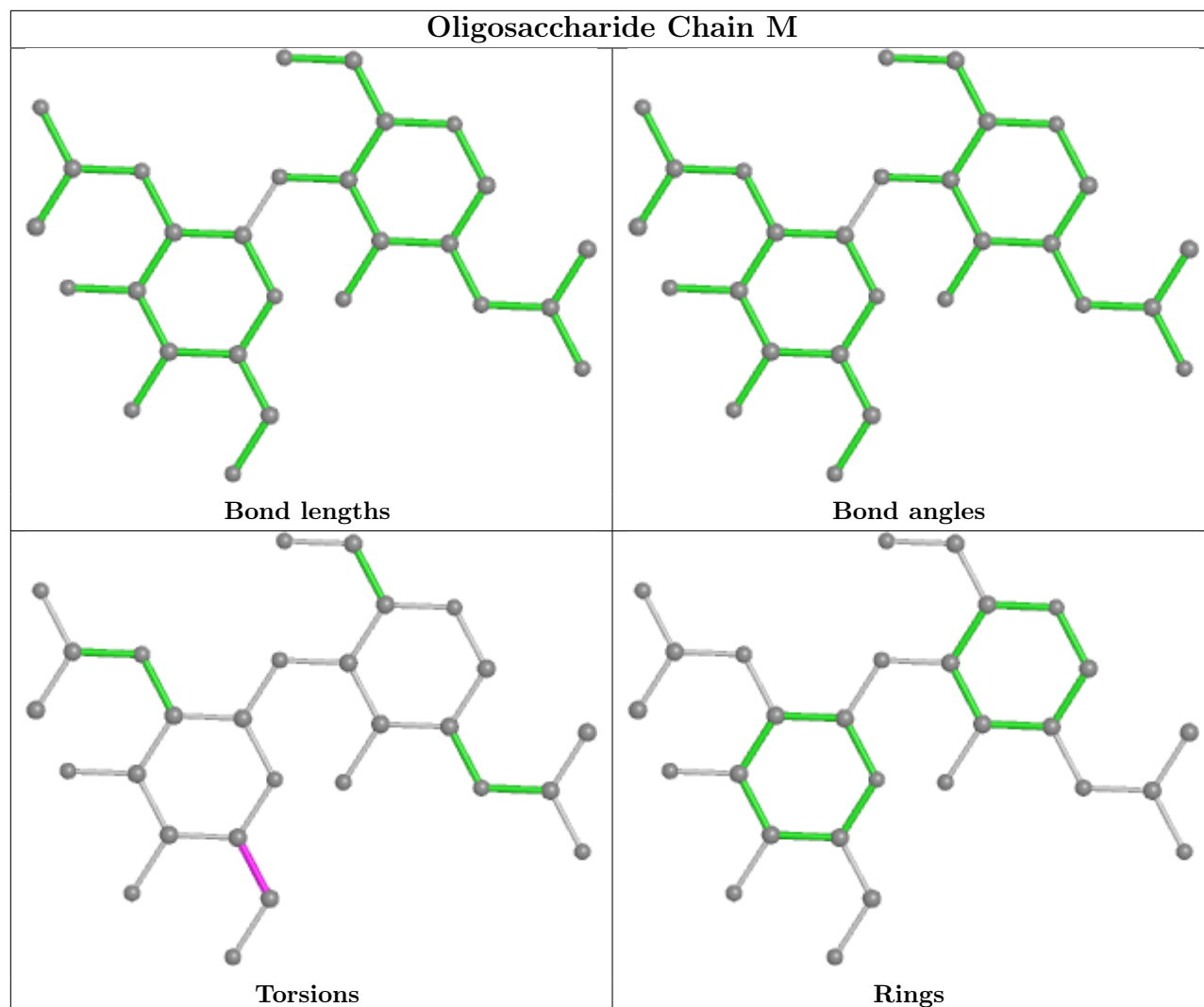
bond angles, torsion angles, and ring geometry for oligosaccharide.

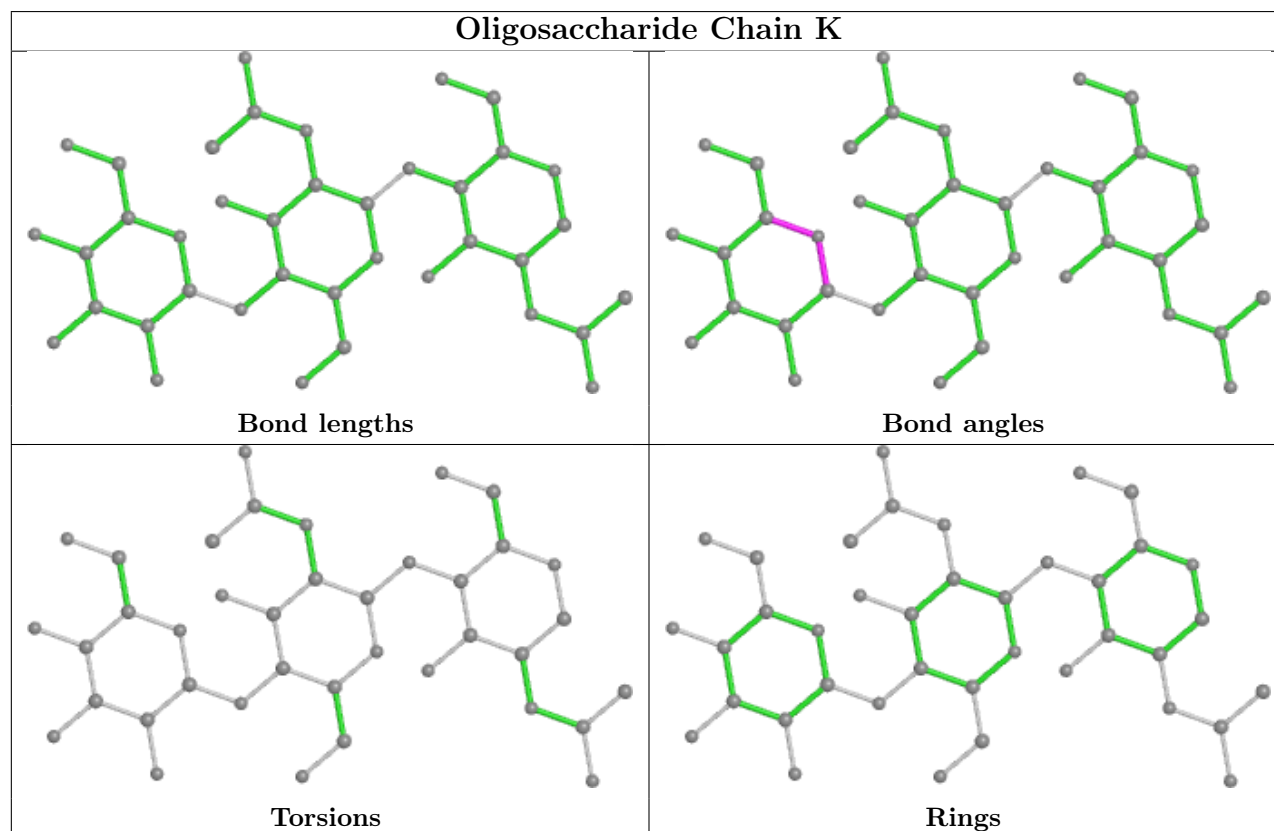
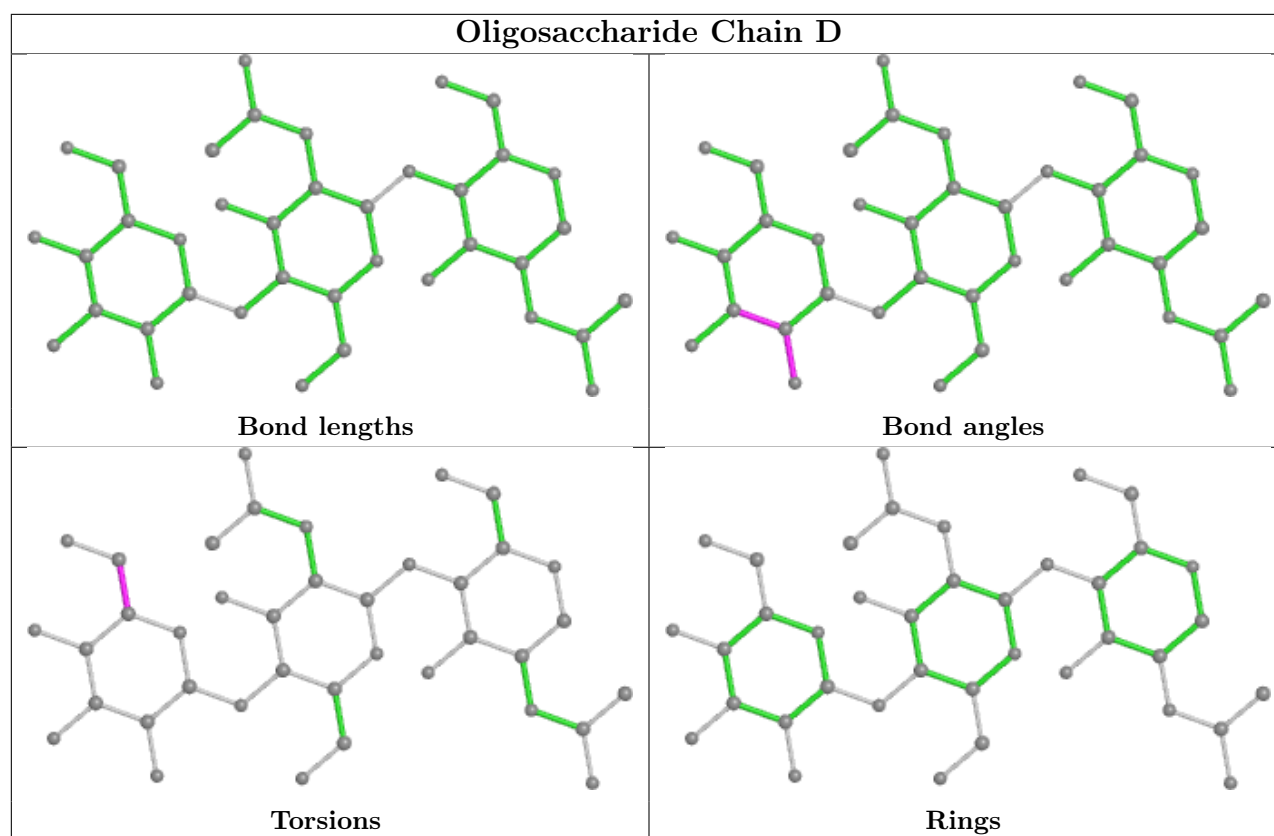


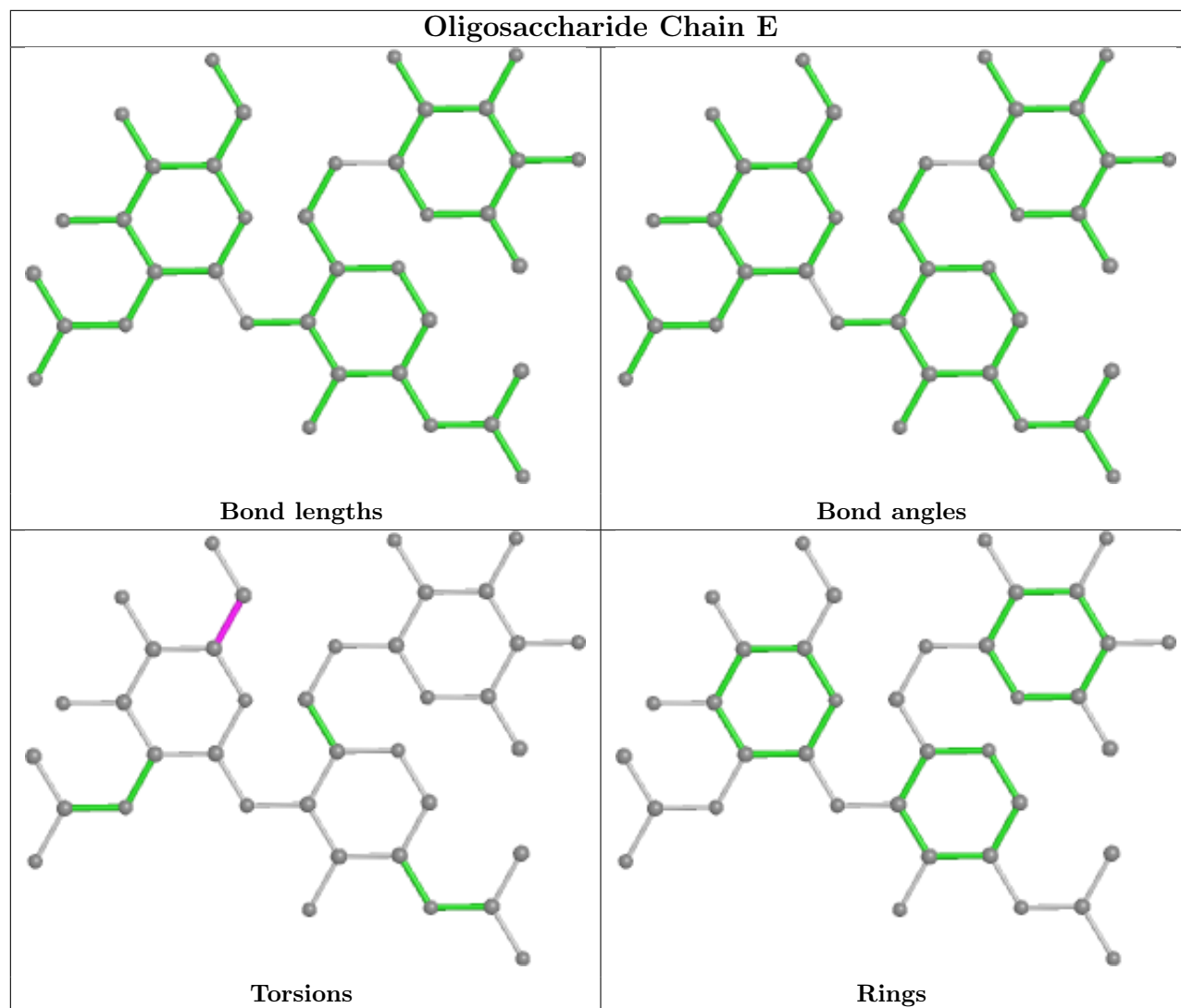


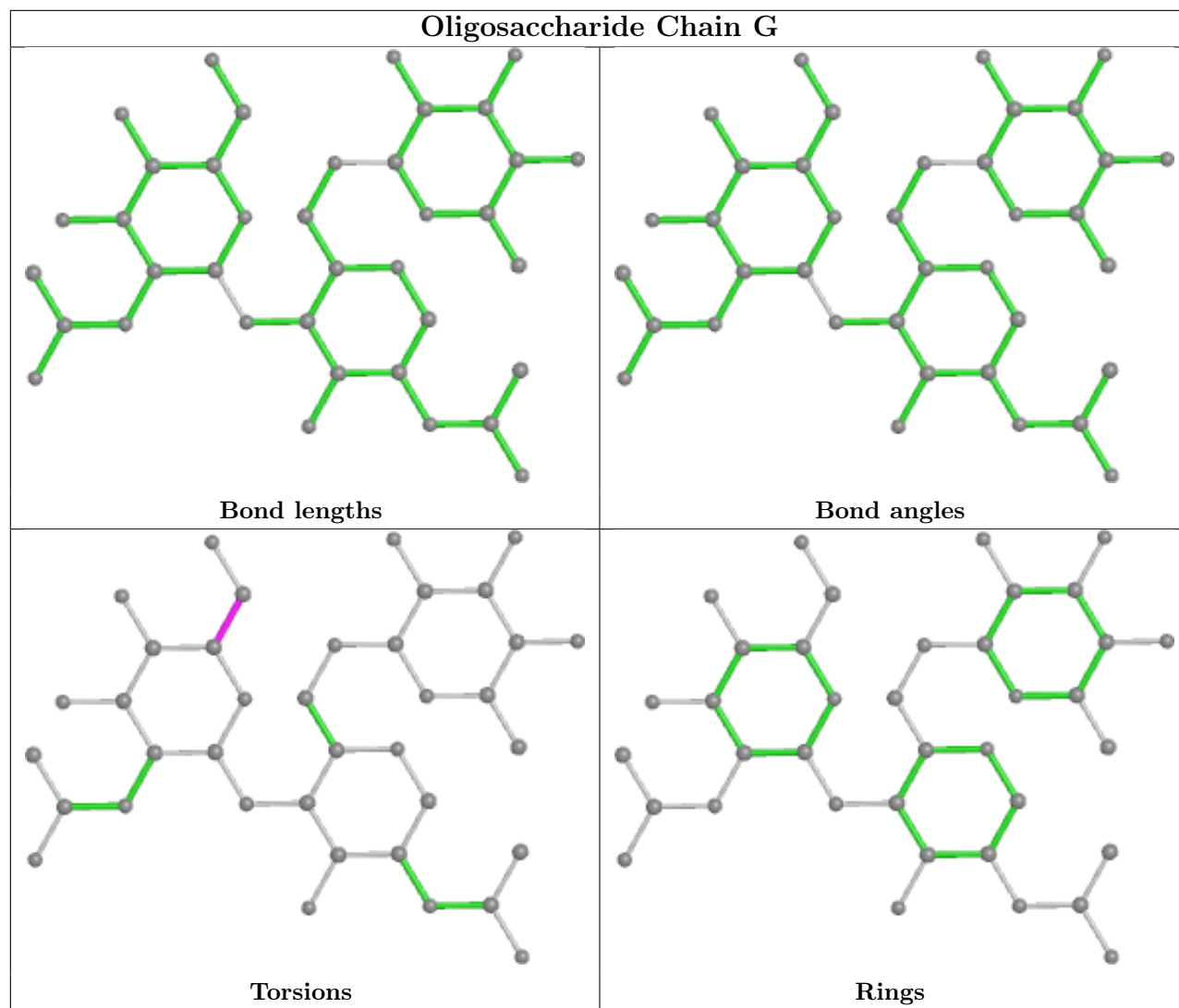


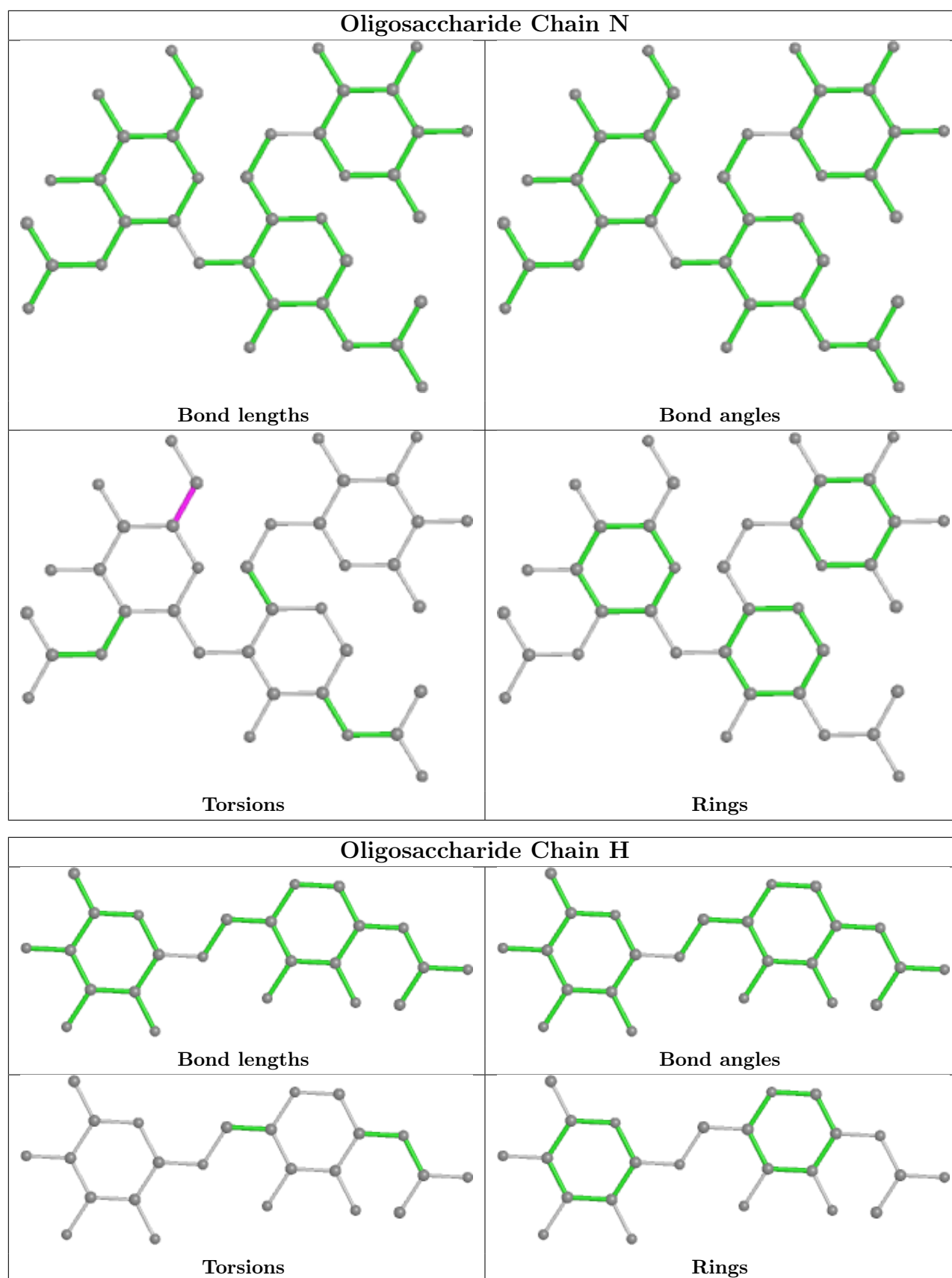


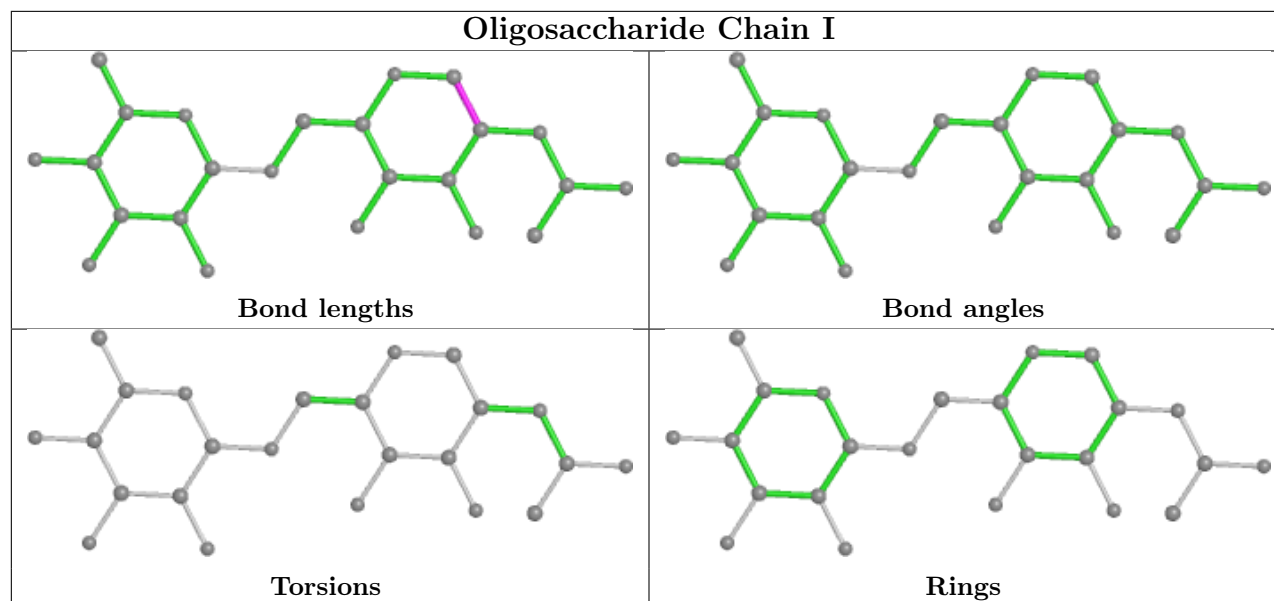












5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 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	APC	A	927	6	27,33,33	4.67	12 (44%)	31,52,52	2.41	6 (19%)
10	SO4	B	918	-	4,4,4	0.13	0	6,6,6	0.09	0
10	SO4	A	925	-	4,4,4	0.13	0	6,6,6	0.19	0
11	APC	B	919	6	27,33,33	4.68	12 (44%)	31,52,52	2.31	6 (19%)
10	SO4	B	917	-	4,4,4	0.13	0	6,6,6	0.19	0
10	SO4	A	926	-	4,4,4	0.13	0	6,6,6	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	APC	A	927	6	-	3/15/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	APC	B	919	6	-	3/15/38/38	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	927	APC	O4'-C1'	15.00	1.62	1.41
11	B	919	APC	O4'-C1'	14.74	1.61	1.41
11	B	919	APC	C2'-C1'	-14.60	1.31	1.53
11	A	927	APC	C2'-C1'	-14.32	1.32	1.53
11	B	919	APC	O4'-C4'	-6.38	1.30	1.45

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	927	APC	C5-C6-N6	8.02	132.54	120.35
11	B	919	APC	C5-C6-N6	7.98	132.48	120.35
11	A	927	APC	N3-C2-N1	-5.73	119.72	128.68
11	B	919	APC	N3-C2-N1	-5.38	120.27	128.68
11	A	927	APC	N6-C6-N1	-5.36	107.46	118.57

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	927	APC	C5'-O5'-PA-O1A
11	B	919	APC	C5'-O5'-PA-O1A
11	B	919	APC	C4'-C5'-O5'-PA
11	A	927	APC	C4'-C5'-O5'-PA
11	A	927	APC	C5'-O5'-PA-O2A

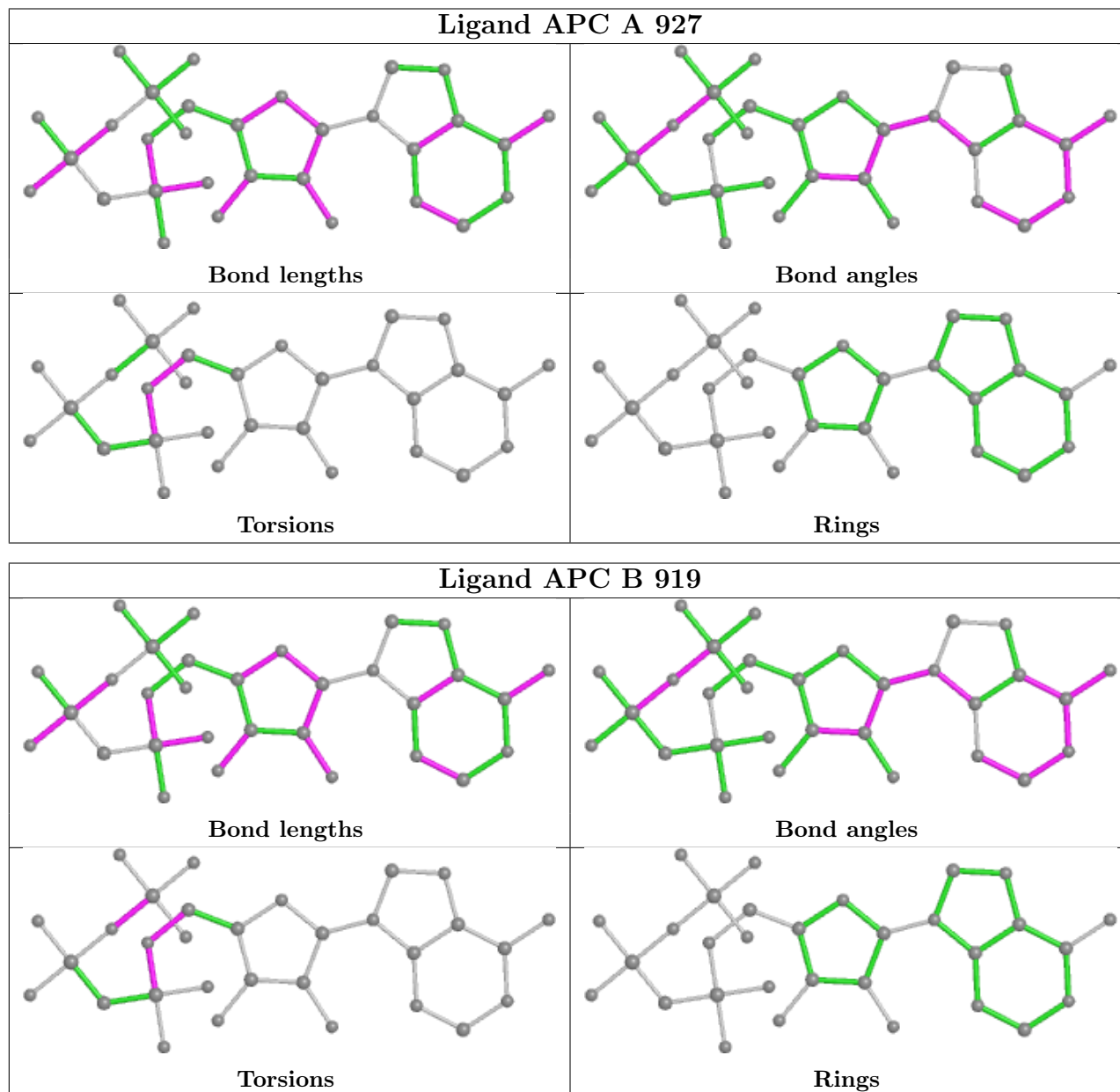
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	927	APC	3	0
11	B	919	APC	2	0

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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	815/838 (97%)	0.06	29 (3%) 42 50	11, 25, 54, 89	0
1	B	815/838 (97%)	0.24	52 (6%) 19 26	11, 30, 75, 107	0
All	All	1630/1676 (97%)	0.15	81 (4%) 28 36	11, 27, 61, 107	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	569	PRO	9.1
1	B	595	LEU	9.0
1	B	568	LEU	8.4
1	B	586	LEU	7.8
1	A	656	PRO	7.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FUC	E	3	10/11	0.69	0.37	46,52,59,62	0
4	NAG	N	2	14/15	0.73	0.21	50,59,68,68	0
2	NAG	L	2	14/15	0.77	0.28	48,51,60,60	0
2	NAG	J	2	14/15	0.79	0.23	43,53,63,68	0
4	NAG	G	2	14/15	0.85	0.15	46,51,61,62	0

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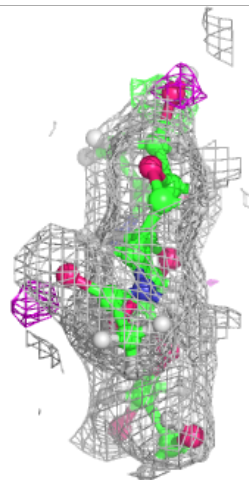
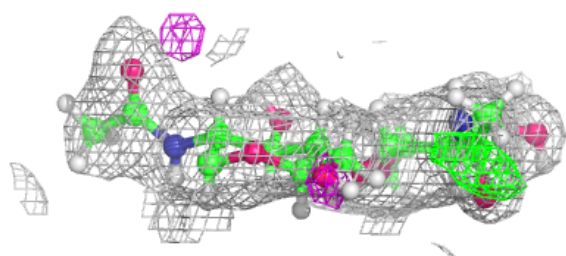
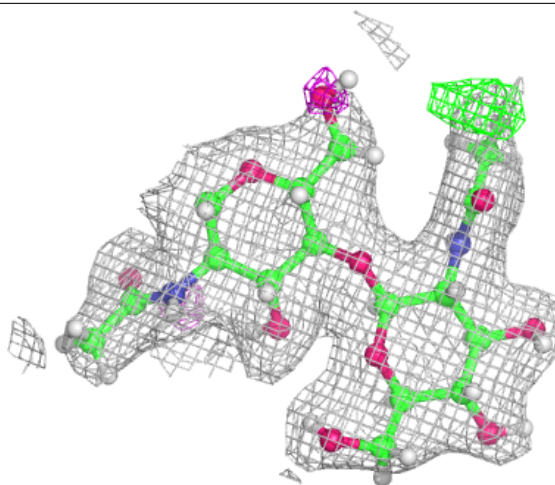
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FUC	G	3	10/11	0.85	0.19	49,57,64,68	0
2	NAG	L	1	14/15	0.85	0.13	37,48,57,57	0
4	NAG	N	1	14/15	0.86	0.14	38,51,63,63	0
4	NAG	G	1	14/15	0.86	0.12	33,46,55,55	0
4	NAG	E	2	14/15	0.87	0.22	39,47,56,60	0
3	BMA	K	3	11/12	0.88	0.09	35,43,50,53	0
3	BMA	D	3	11/12	0.88	0.12	29,39,50,54	0
2	NAG	M	2	14/15	0.89	0.11	32,42,52,60	0
4	NAG	E	1	14/15	0.89	0.13	29,38,46,50	0
2	NAG	F	2	14/15	0.89	0.13	32,43,52,55	0
5	NAG	I	1	14/15	0.89	0.12	27,37,43,47	0
5	NAG	H	1	14/15	0.90	0.12	36,48,57,61	0
2	NAG	C	2	14/15	0.90	0.10	40,48,61,62	0
5	FUC	H	2	10/11	0.91	0.10	41,48,57,57	0
2	NAG	C	1	14/15	0.92	0.12	23,32,43,49	0
2	NAG	J	1	14/15	0.92	0.13	27,38,54,56	0
4	FUC	N	3	10/11	0.92	0.13	37,43,51,52	0
3	NAG	D	1	14/15	0.95	0.11	15,22,30,38	0
5	FUC	I	2	10/11	0.95	0.10	32,39,44,47	0
3	NAG	K	2	14/15	0.96	0.07	19,25,31,33	0
3	NAG	D	2	14/15	0.96	0.07	15,23,29,34	0
3	NAG	K	1	14/15	0.96	0.10	15,22,26,31	0
2	NAG	F	1	14/15	0.97	0.09	13,18,23,26	0
2	NAG	M	1	14/15	0.97	0.09	15,19,23,24	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.

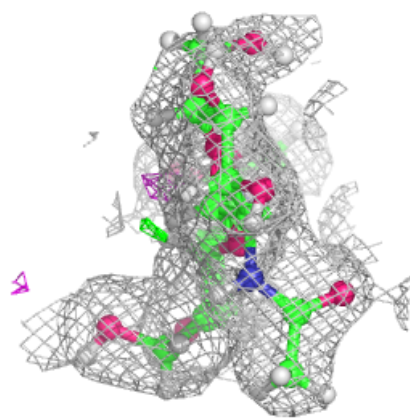
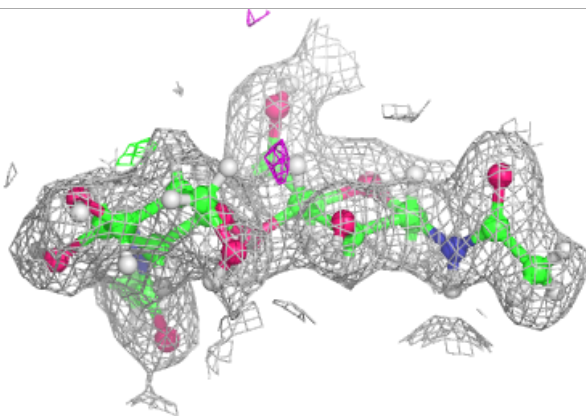
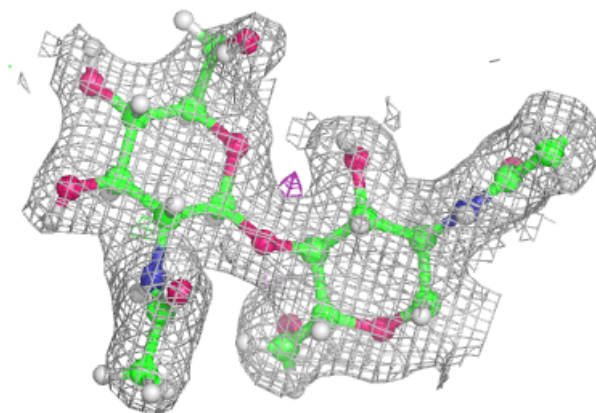
Electron density around Chain C:

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



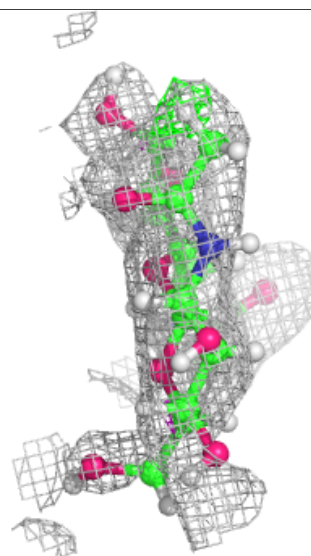
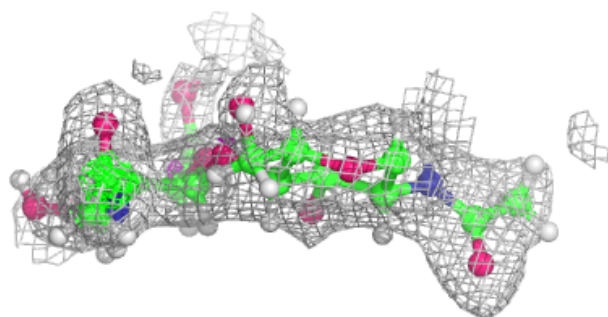
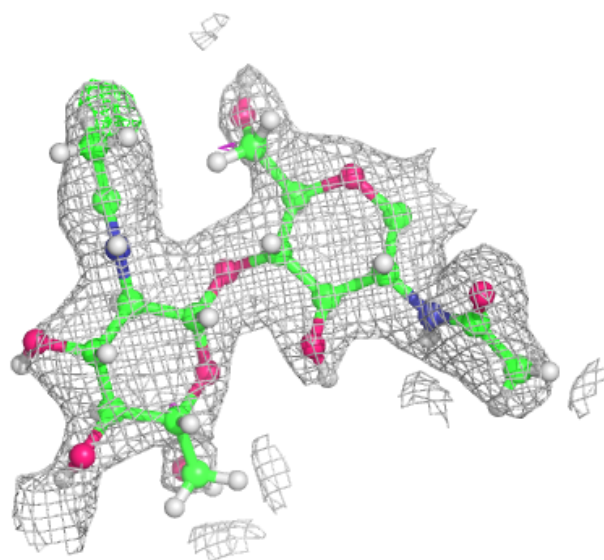
Electron density around Chain F:

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and green (positive)



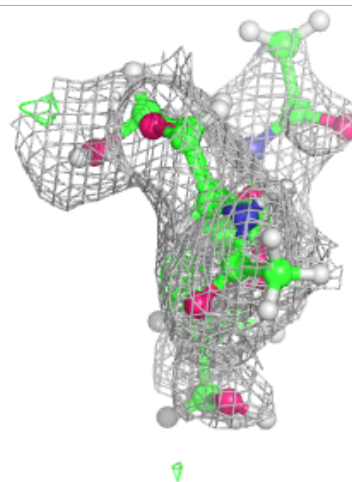
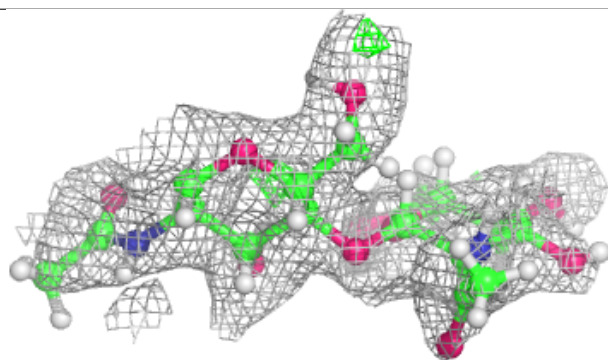
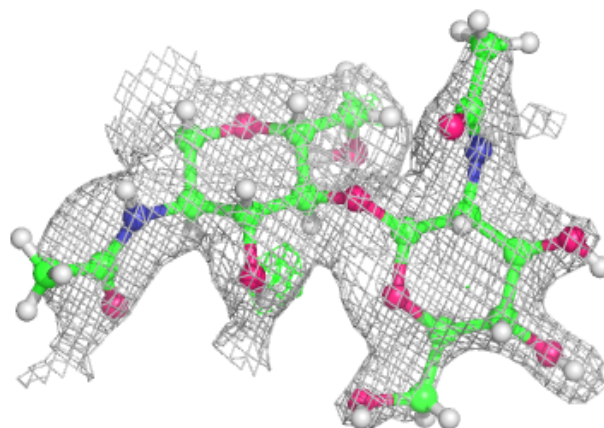
Electron density around Chain J:

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



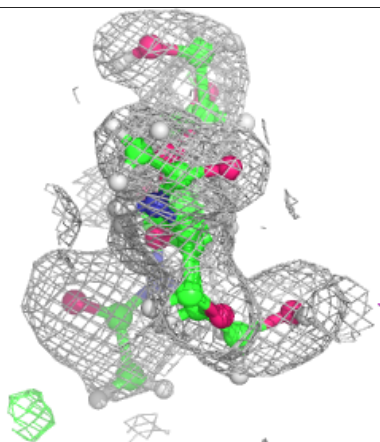
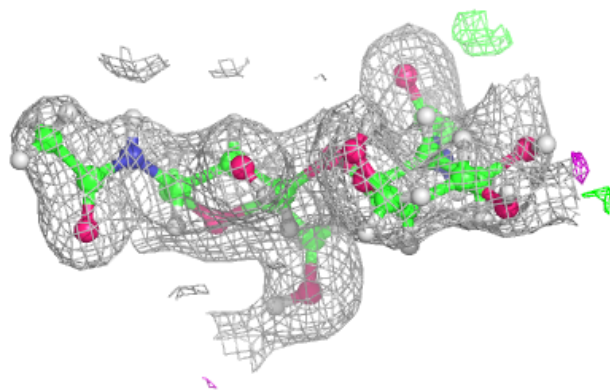
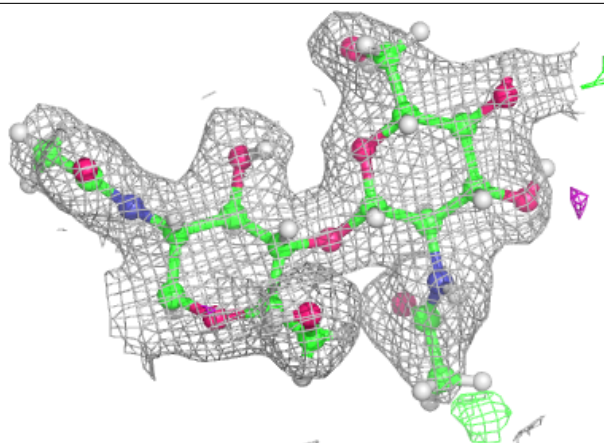
Electron density around Chain L:

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

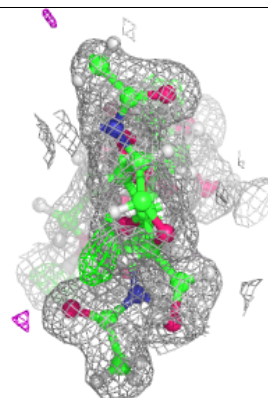
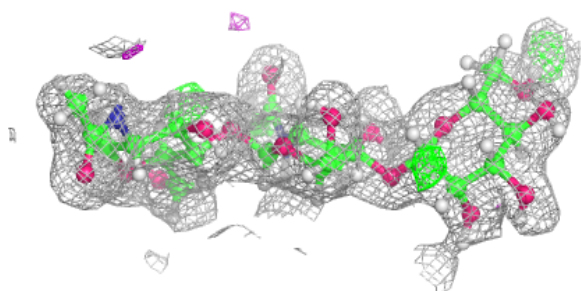
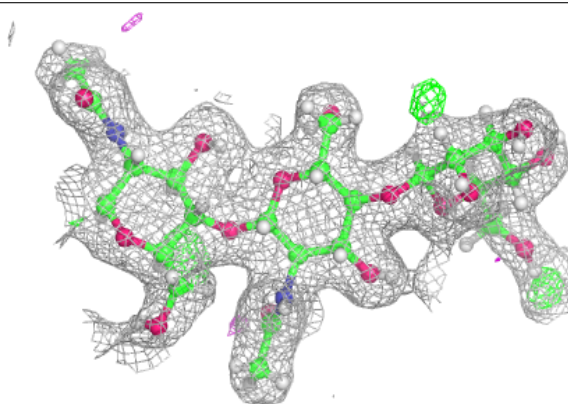


Electron density around Chain M:

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

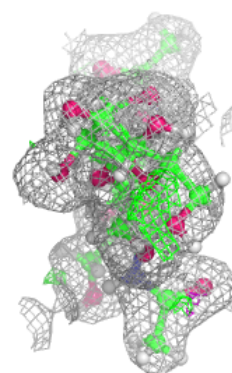
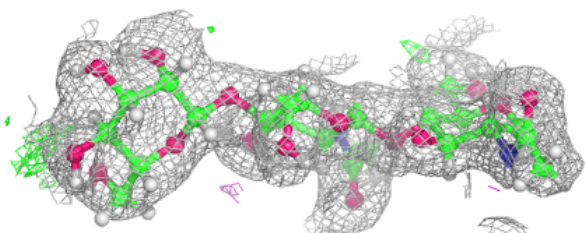
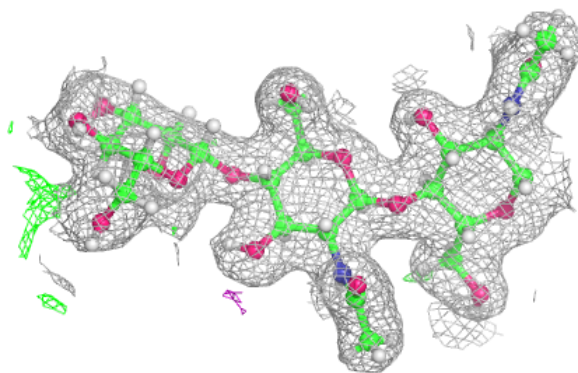
**Electron density around Chain D:**

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



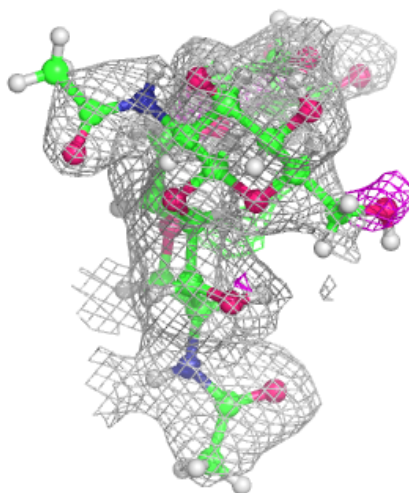
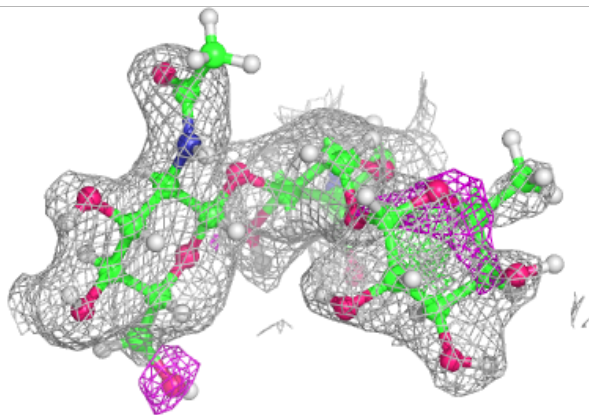
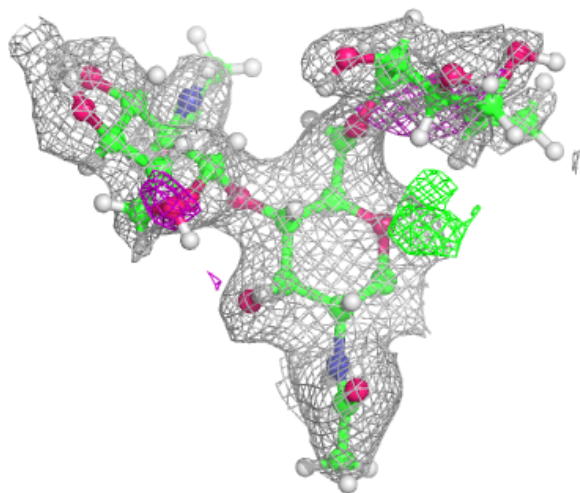
Electron density around Chain K:

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



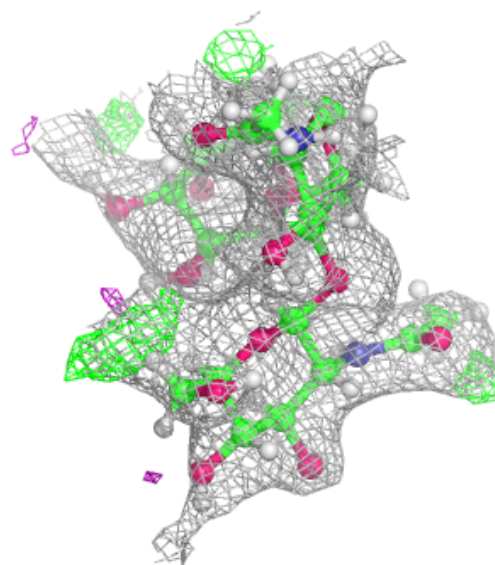
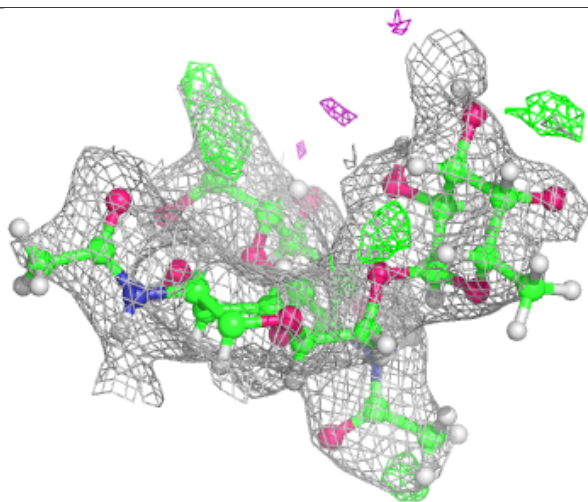
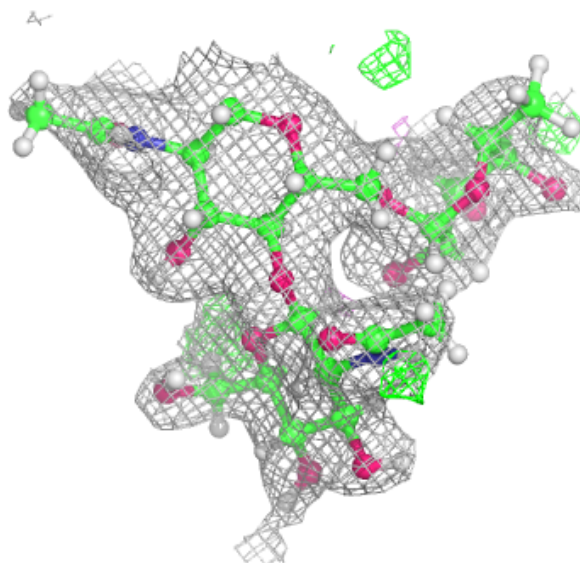
Electron density around Chain E:

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



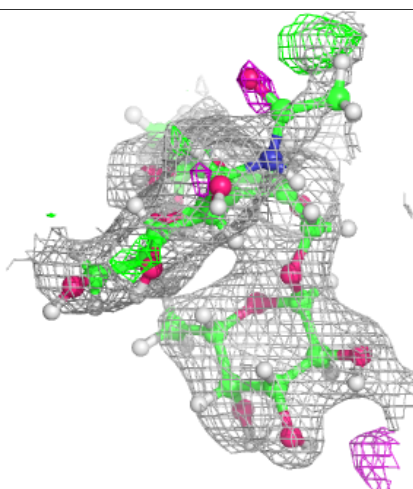
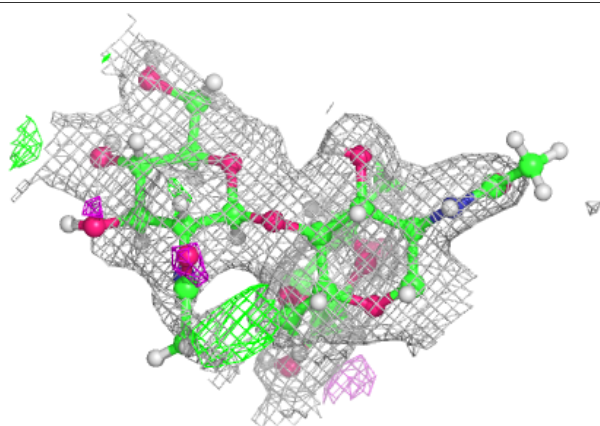
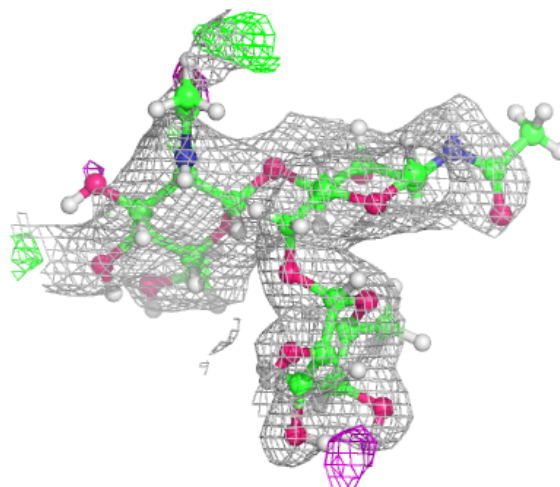
Electron density around Chain G:

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



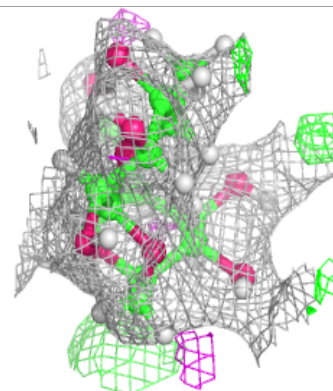
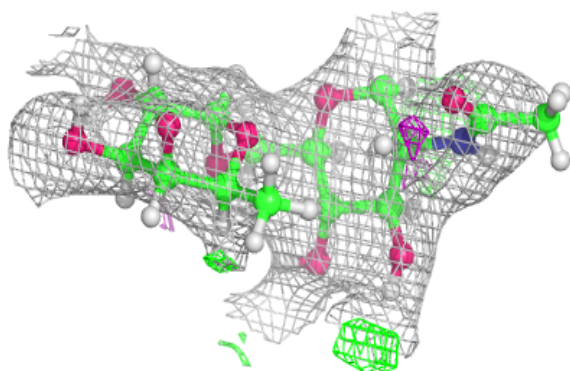
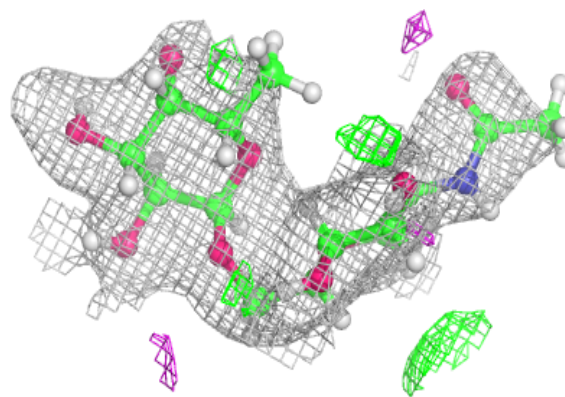
Electron density around Chain N:

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

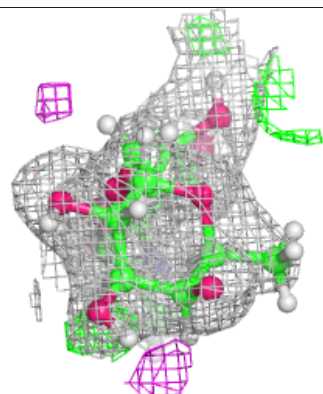
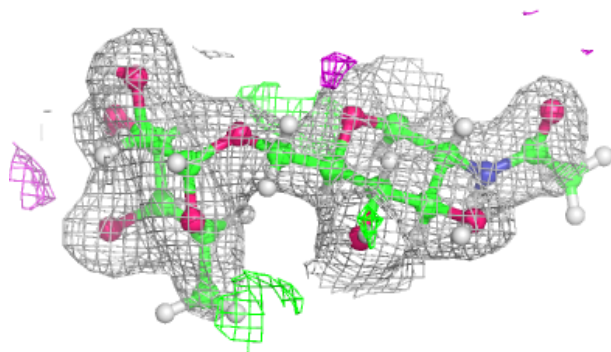
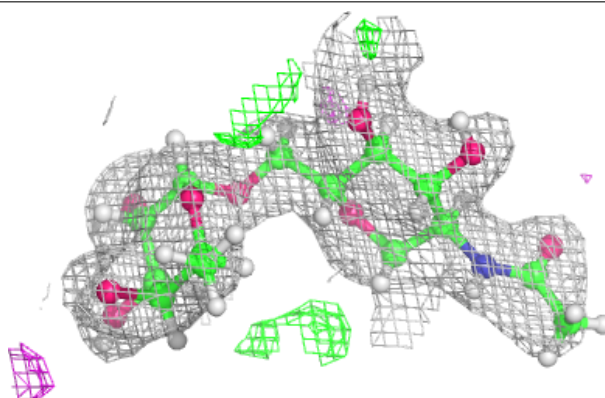


Electron density around Chain H:

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

**Electron density around Chain I:**

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

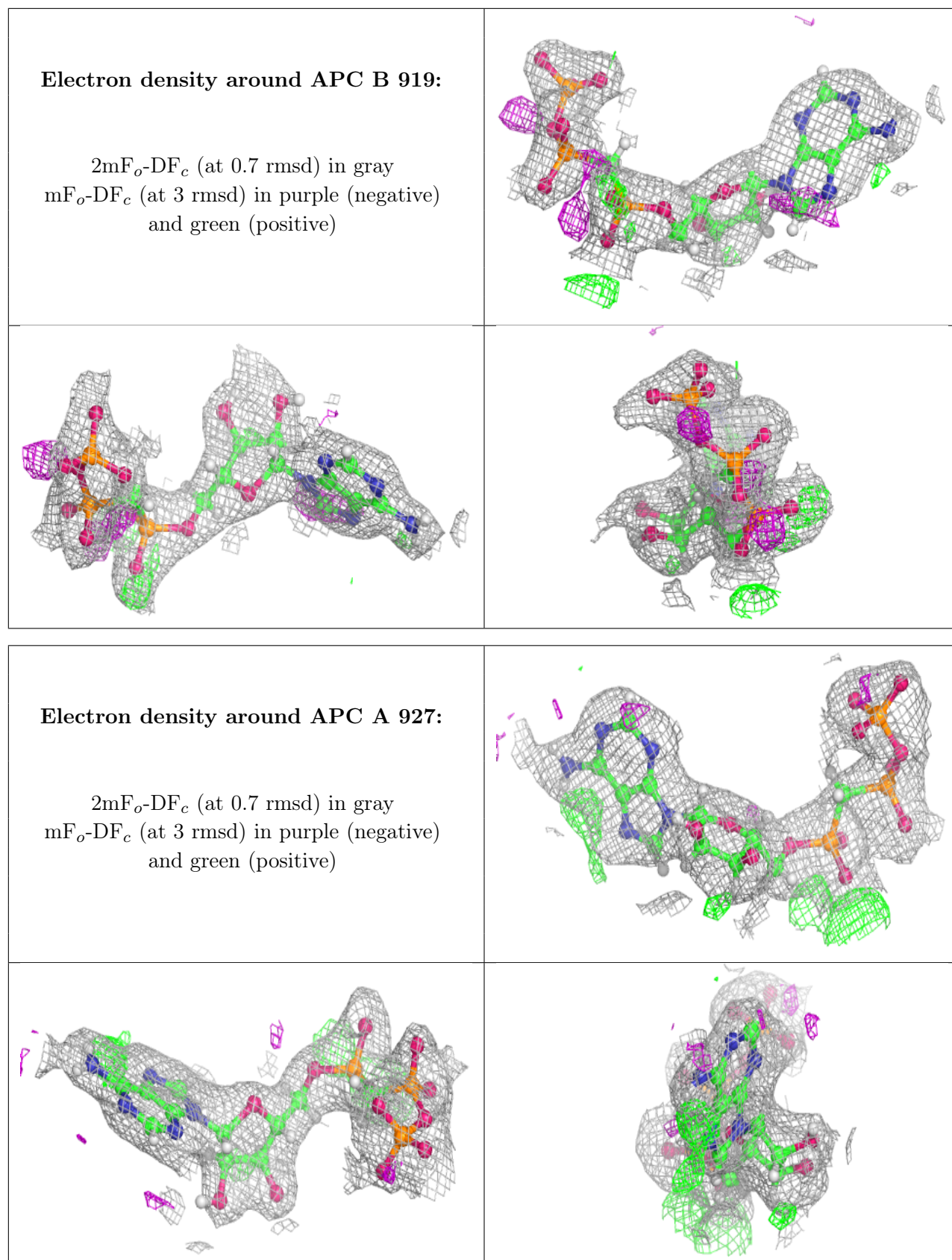


6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NA	B	916	1/1	0.91	0.11	38,38,38,38	0
11	APC	B	919	31/31	0.91	0.12	28,36,46,51	0
10	SO4	A	926	5/5	0.92	0.13	48,50,51,51	0
9	CL	A	923	1/1	0.92	0.08	42,42,42,42	0
11	APC	A	927	31/31	0.93	0.11	22,33,46,49	0
9	CL	A	924	1/1	0.93	0.06	74,74,74,74	0
9	CL	A	922	1/1	0.94	0.19	65,65,65,65	0
8	NA	A	921	1/1	0.94	0.09	40,40,40,40	0
6	ZN	A	902	1/1	0.95	0.12	19,19,19,19	1
10	SO4	B	917	5/5	0.96	0.12	43,46,47,47	0
7	CA	A	903	1/1	0.97	0.33	52,52,52,52	0
10	SO4	B	918	5/5	0.97	0.11	49,49,50,51	0
10	SO4	A	925	5/5	0.98	0.07	36,38,40,40	0
6	ZN	B	902	1/1	0.98	0.09	29,29,29,29	1
7	CA	B	903	1/1	0.99	0.09	22,22,22,22	0
6	ZN	A	901	1/1	0.99	0.24	41,41,41,41	0
6	ZN	B	901	1/1	0.99	0.16	31,31,31,31	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.