



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:06 PM BST

PDB ID : 5BO7  
Title : Structure of human sialyltransferase ST8SiaIII in complex with CTP  
Authors : Volkers, G.; Worrall, L.; Strynadka, N.C.J.  
Deposited on : 2015-05-27  
Resolution : 1.85 Å(reported)

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

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

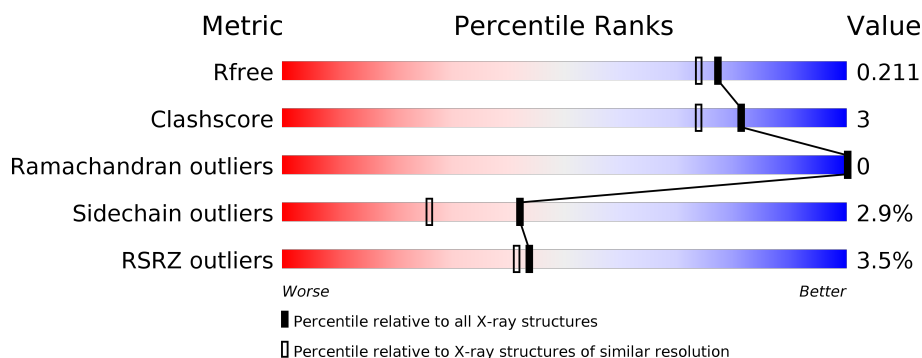
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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.



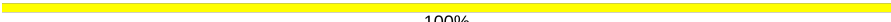
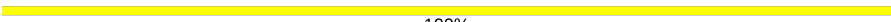
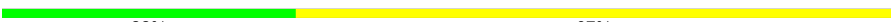
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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	323	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>5%</div> <div>10%</div> </div> </div>
1	B	323	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div>14%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>
2	G	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
2	I	2	 100%
3	E	3	 33% 67%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5314 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sia-alpha-2,3-Gal-beta-1,4-GlcNAc-R:alpha 2,8-sialyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2369	1531	410	418	10			
1	B	279	Total	C	N	O	S	0	1	0
			2303	1488	400	405	10			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	ALA	-	expression tag	UNP O43173
A	59	PRO	-	expression tag	UNP O43173
A	60	GLU	-	expression tag	UNP O43173
A	61	HIS	-	expression tag	UNP O43173
A	62	HIS	-	expression tag	UNP O43173
A	63	HIS	-	expression tag	UNP O43173
A	64	HIS	-	expression tag	UNP O43173
A	65	HIS	-	expression tag	UNP O43173
A	66	HIS	-	expression tag	UNP O43173
A	67	ASP	-	expression tag	UNP O43173
A	68	TYR	-	expression tag	UNP O43173
A	69	ASP	-	expression tag	UNP O43173
A	70	ILE	-	expression tag	UNP O43173
A	71	PRO	-	expression tag	UNP O43173
A	72	THR	-	expression tag	UNP O43173
A	73	THR	-	expression tag	UNP O43173
A	74	GLU	-	expression tag	UNP O43173
A	75	ASN	-	expression tag	UNP O43173
A	76	LEU	-	expression tag	UNP O43173
A	77	TYR	-	expression tag	UNP O43173
A	78	PHE	-	expression tag	UNP O43173
A	79	GLN	-	expression tag	UNP O43173
A	80	GLY	-	expression tag	UNP O43173
B	58	ALA	-	expression tag	UNP O43173

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Chain	Residue	Modelled	Actual	Comment	Reference
B	59	PRO	-	expression tag	UNP O43173
B	60	GLU	-	expression tag	UNP O43173
B	61	HIS	-	expression tag	UNP O43173
B	62	HIS	-	expression tag	UNP O43173
B	63	HIS	-	expression tag	UNP O43173
B	64	HIS	-	expression tag	UNP O43173
B	65	HIS	-	expression tag	UNP O43173
B	66	HIS	-	expression tag	UNP O43173
B	67	ASP	-	expression tag	UNP O43173
B	68	TYR	-	expression tag	UNP O43173
B	69	ASP	-	expression tag	UNP O43173
B	70	ILE	-	expression tag	UNP O43173
B	71	PRO	-	expression tag	UNP O43173
B	72	THR	-	expression tag	UNP O43173
B	73	THR	-	expression tag	UNP O43173
B	74	GLU	-	expression tag	UNP O43173
B	75	ASN	-	expression tag	UNP O43173
B	76	LEU	-	expression tag	UNP O43173
B	77	TYR	-	expression tag	UNP O43173
B	78	PHE	-	expression tag	UNP O43173
B	79	GLN	-	expression tag	UNP O43173
B	80	GLY	-	expression tag	UNP O43173

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



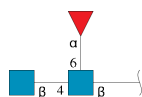
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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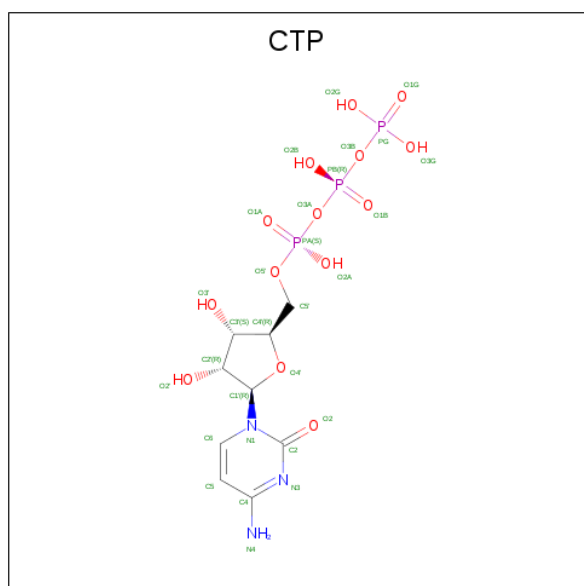
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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
3	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula:  $C_9H_{16}N_3O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

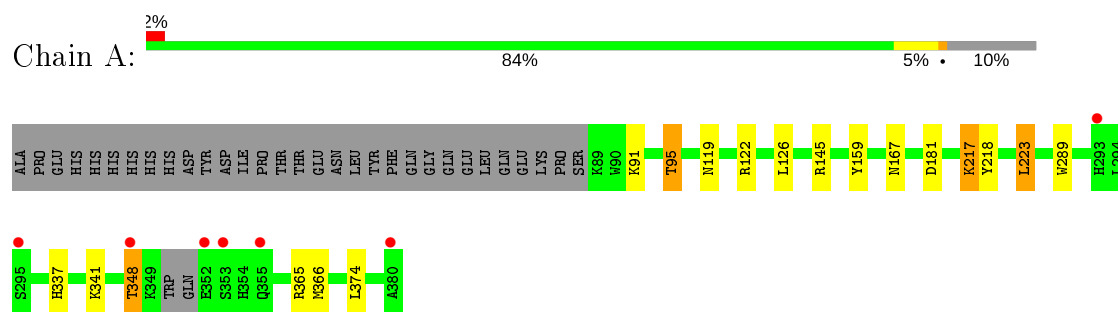
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	214	Total	O	0	0
			214	214		
6	B	150	Total	O	0	0
			150	150		

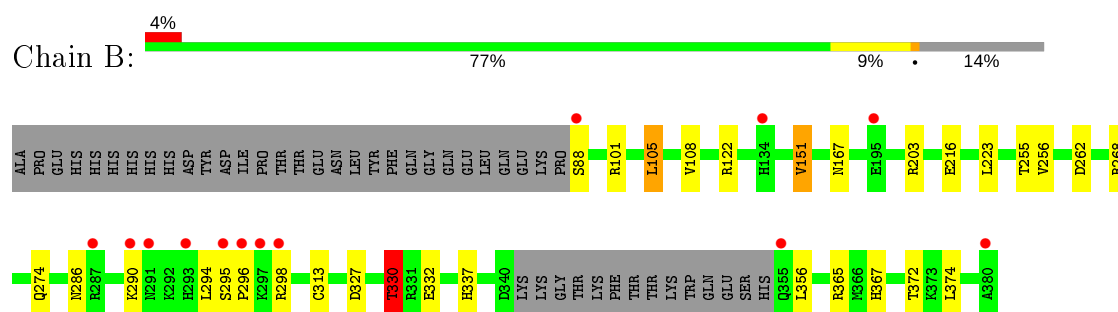
### 3 Residue-property plots [i](#)

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.

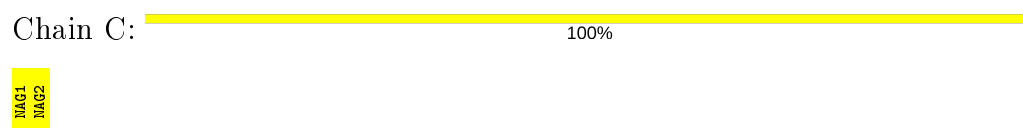
- Molecule 1: Sia-alpha-2,3-Gal-beta-1,4-GlcNAc-R:alpha 2,8-sialyltransferase



- Molecule 1: Sia-alpha-2,3-Gal-beta-1,4-GlcNAc-R:alpha 2,8-sialyltransferase



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



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






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

Chain F:  100%

NAG1  
NAG2

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

Chain G:  100%

NAG1  
NAG2

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

Chain H:  100%

NAG1  
NAG2

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

Chain I:  100%

NAG1  
NAG2

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

Chain E:  33% 67%

NAG1  
NAG2  
FUC3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.33 Å 96.50 Å 124.66 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.94 – 1.85 46.94 – 1.85	Depositor EDS
% Data completeness (in resolution range)	95.2 (46.94-1.85) 95.2 (46.94-1.85)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.86 Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, $R_{free}$	0.170 , 0.200 0.179 , 0.211	Depositor DCC
$R_{free}$ test set	3484 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5314	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CTP, NAG, FUC

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	1.06	2/2437 (0.1%)	0.96	6/3303 (0.2%)
1	B	0.98	0/2372	0.97	8/3214 (0.2%)
All	All	1.02	2/4809 (0.0%)	0.96	14/6517 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	TYR	CE1-CZ	-5.23	1.31	1.38
1	A	289	TRP	CG-CD1	-5.14	1.29	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	LEU	CA-CB-CG	8.34	134.48	115.30
1	A	122	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	330	THR	N-CA-CB	-6.82	97.34	110.30
1	B	151	VAL	CG1-CB-CG2	6.76	121.72	110.90
1	A	223	LEU	CB-CG-CD1	6.31	121.72	111.00
1	B	262	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	374	LEU	CA-CB-CG	5.75	128.53	115.30
1	A	122	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	181	ASP	CB-CG-OD1	5.61	123.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	VAL	CA-CB-CG2	5.57	119.25	110.90
1	B	268	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	B	365	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	108	VAL	CB-CA-C	-5.34	101.25	111.40
1	A	126	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	294	LEU	Peptide
1	B	88	SER	Peptide

## 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	2369	0	2291	9	0
1	B	2303	0	2243	16	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	E	38	0	34	0	0
4	A	29	0	12	0	0
4	B	29	0	12	0	0
5	B	14	0	13	0	0
6	A	214	0	0	9	0
6	B	150	0	0	2	0
All	All	5314	0	4755	25	0

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

All (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:366:MET:SD	6:A:686:HOH:O	2.16	1.02
1:B:367:HIS:HD2	1:B:374:LEU:H	1.29	0.78
1:B:330:THR:HG21	6:B:639:HOH:O	1.85	0.77
6:A:506:HOH:O	1:B:223:LEU:HD22	1.84	0.75
1:B:367:HIS:CD2	1:B:374:LEU:H	2.08	0.72
1:B:330:THR:HG23	1:B:332:GLU:HG2	1.74	0.69
6:A:611:HOH:O	1:B:255:THR:HG22	1.93	0.68
1:B:101:ARG:NH2	1:B:313:CYS:O	2.27	0.67
1:A:119:ASN:HB2	6:A:622:HOH:O	1.97	0.64
1:A:95:THR:HG21	6:A:700:HOH:O	1.98	0.62
1:B:327:ASP:HB3	1:B:330:THR:HG22	1.83	0.61
1:A:95:THR:HG23	6:A:674:HOH:O	2.07	0.55
1:B:216:GLU:HG3	1:B:256:VAL:HG11	1.88	0.55
1:B:274:GLN:HG3	6:B:598:HOH:O	2.08	0.53
1:B:330:THR:HG23	1:B:332:GLU:CG	2.39	0.52
1:B:330:THR:CG2	1:B:332:GLU:H	2.24	0.51
1:B:330:THR:HG22	1:B:332:GLU:H	1.76	0.50
1:A:217:LYS:HD2	1:A:218:TYR:CZ	2.48	0.48
1:A:365:ARG:NH1	6:A:505:HOH:O	2.40	0.46
1:A:348:THR:HA	6:A:683:HOH:O	2.14	0.46
1:B:295:SER:N	1:B:296:PRO:CD	2.80	0.45
1:B:167:ASN:O	1:B:337:HIS:HA	2.17	0.43
1:A:145:ARG:NH1	6:A:510:HOH:O	2.49	0.43
1:A:167:ASN:O	1:A:337:HIS:HA	2.20	0.42
1:B:367:HIS:HA	1:B:372:THR:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	286/323 (88%)	282 (99%)	4 (1%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	276/323 (85%)	272 (99%)	4 (1%)	0	100	100
All	All	562/646 (87%)	554 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/294 (87%)	251 (98%)	6 (2%)	50	34
1	B	253/294 (86%)	244 (96%)	9 (4%)	35	18
All	All	510/588 (87%)	495 (97%)	15 (3%)	42	26

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LYS
1	A	95	THR
1	A	217	LYS
1	A	223	LEU
1	A	341	LYS
1	A	348	THR
1	B	105	LEU
1	B	122	ARG
1	B	151	VAL
1	B	203	ARG
1	B	286	ASN
1	B	290	LYS
1	B	298	ARG
1	B	330	THR
1	B	356	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	134	HIS
1	B	134	HIS
1	B	267	HIS
1	B	355	GLN
1	B	367	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

15 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	0.44	0	17,19,21	1.27	1 (5%)
2	NAG	C	2	2	14,14,15	0.68	0	17,19,21	1.66	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.56	0	17,19,21	1.09	0
2	NAG	D	2	2	14,14,15	0.33	0	17,19,21	0.97	1 (5%)
3	NAG	E	1	1,3	14,14,15	0.75	0	17,19,21	1.10	1 (5%)
3	NAG	E	2	3	14,14,15	0.78	0	17,19,21	1.49	4 (23%)
3	FUC	E	3	3	10,10,11	0.51	0	14,14,16	0.91	0
2	NAG	F	1	1,2	14,14,15	1.00	1 (7%)	17,19,21	1.56	4 (23%)
2	NAG	F	2	2	14,14,15	0.56	0	17,19,21	1.13	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.63	0	17,19,21	1.31	2 (11%)
2	NAG	G	2	2	14,14,15	0.55	0	17,19,21	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	H	1	1,2	14,14,15	0.85	1 (7%)	17,19,21	1.64	3 (17%)
2	NAG	H	2	2	14,14,15	0.48	0	17,19,21	1.24	2 (11%)
2	NAG	I	1	1,2	14,14,15	0.37	0	17,19,21	1.63	3 (17%)
2	NAG	I	2	2	14,14,15	0.28	0	17,19,21	0.77	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	FUC	E	3	3	-	-	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C8-C7	-2.61	1.45	1.50
2	H	1	NAG	C2-N2	-2.15	1.42	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	5.06	119.05	112.19
2	I	1	NAG	O5-C1-C2	-3.95	105.05	111.29
2	H	1	NAG	C1-O5-C5	3.88	117.45	112.19
2	F	1	NAG	C2-N2-C7	3.75	128.24	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	O5-C1-C2	-3.53	105.71	111.29
2	I	1	NAG	C8-C7-N2	3.16	121.44	116.10
3	E	1	NAG	C1-C2-N2	3.04	115.68	110.49
2	H	2	NAG	O5-C5-C6	3.03	111.96	107.20
2	G	1	NAG	C1-C2-N2	3.00	115.62	110.49
2	D	2	NAG	O5-C5-C6	2.91	111.76	107.20
3	E	2	NAG	O5-C1-C2	-2.53	107.29	111.29
2	F	1	NAG	O5-C5-C6	2.52	111.16	107.20
2	F	1	NAG	C1-O5-C5	2.46	115.53	112.19
3	E	2	NAG	O5-C5-C6	2.44	111.02	107.20
3	E	2	NAG	C1-C2-N2	-2.37	106.44	110.49
2	C	1	NAG	O6-C6-C5	-2.37	103.18	111.29
3	E	2	NAG	C3-C4-C5	-2.34	106.07	110.24
2	G	1	NAG	O5-C5-C6	2.31	110.83	107.20
2	F	2	NAG	O5-C5-C4	-2.31	105.22	110.83
2	G	2	NAG	O5-C5-C6	2.19	110.63	107.20
2	I	1	NAG	O5-C5-C6	2.14	110.55	107.20
2	H	1	NAG	O4-C4-C3	-2.11	105.46	110.35
2	G	2	NAG	C1-C2-N2	-2.10	106.89	110.49
2	C	2	NAG	O3-C3-C4	-2.09	105.51	110.35
2	I	2	NAG	C1-O5-C5	2.08	115.00	112.19
2	H	2	NAG	C1-O5-C5	-2.03	109.44	112.19
2	F	1	NAG	O4-C4-C5	-2.01	104.31	109.30

There are no chirality outliers.

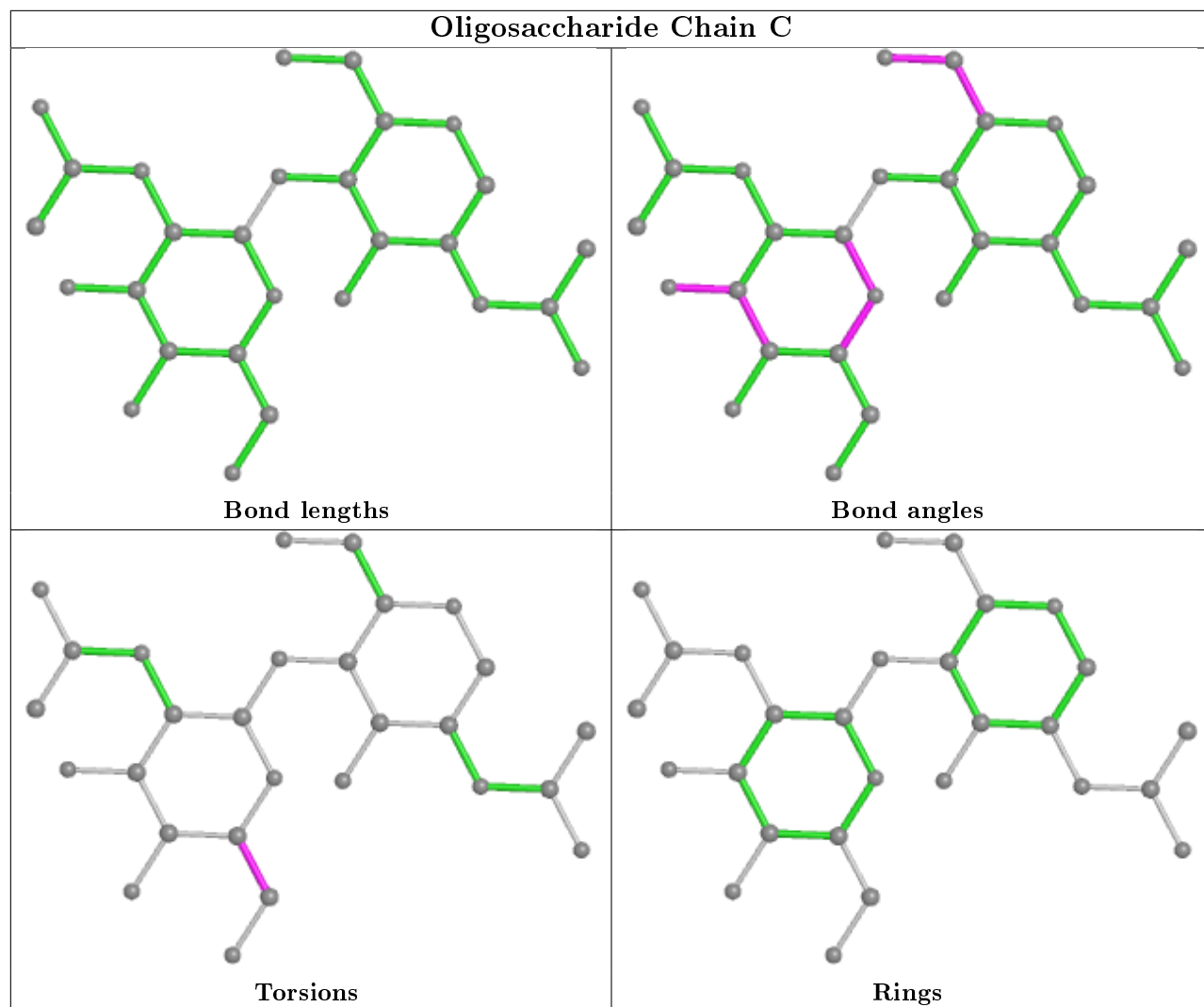
All (8) torsion outliers are listed below:

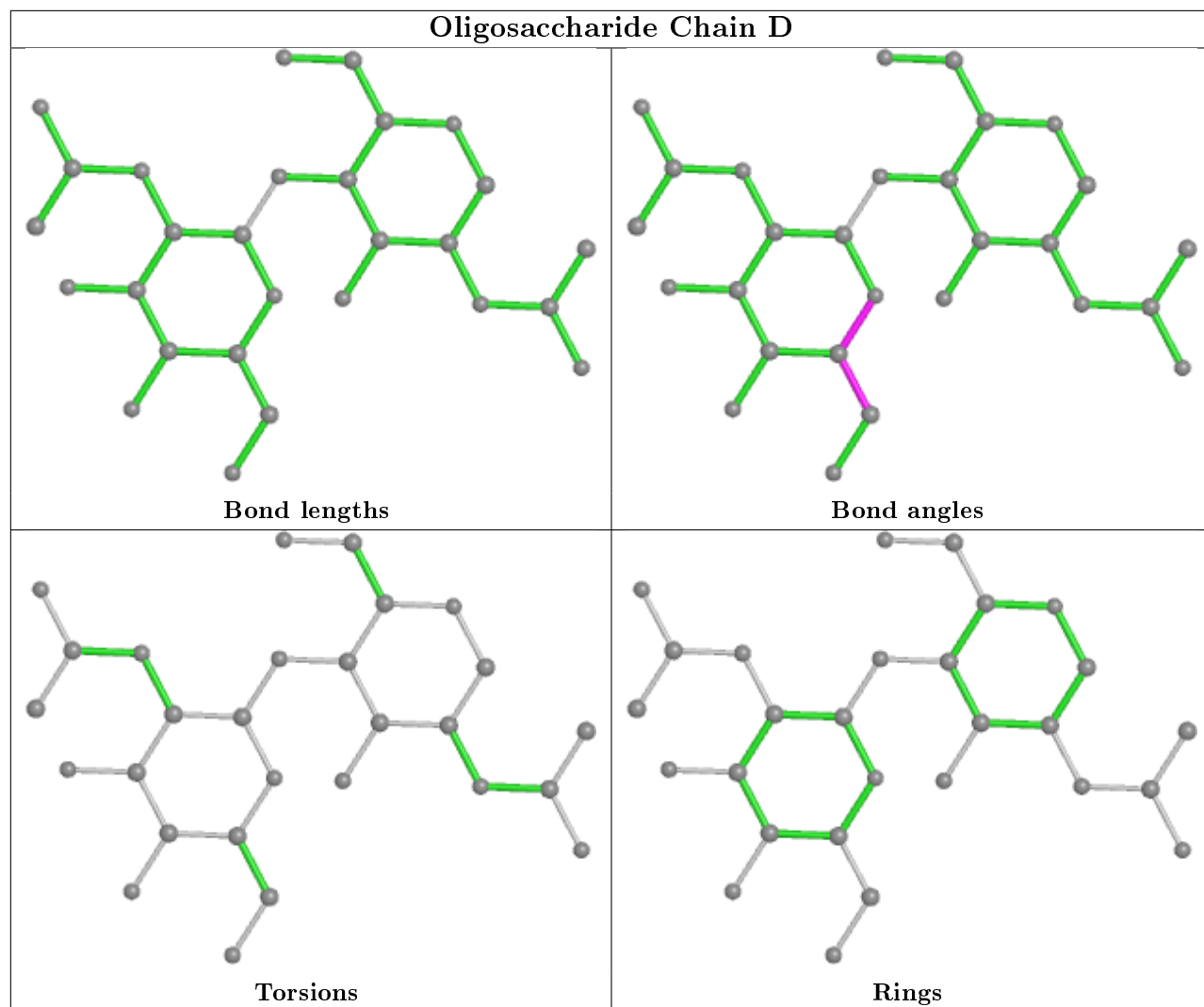
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6

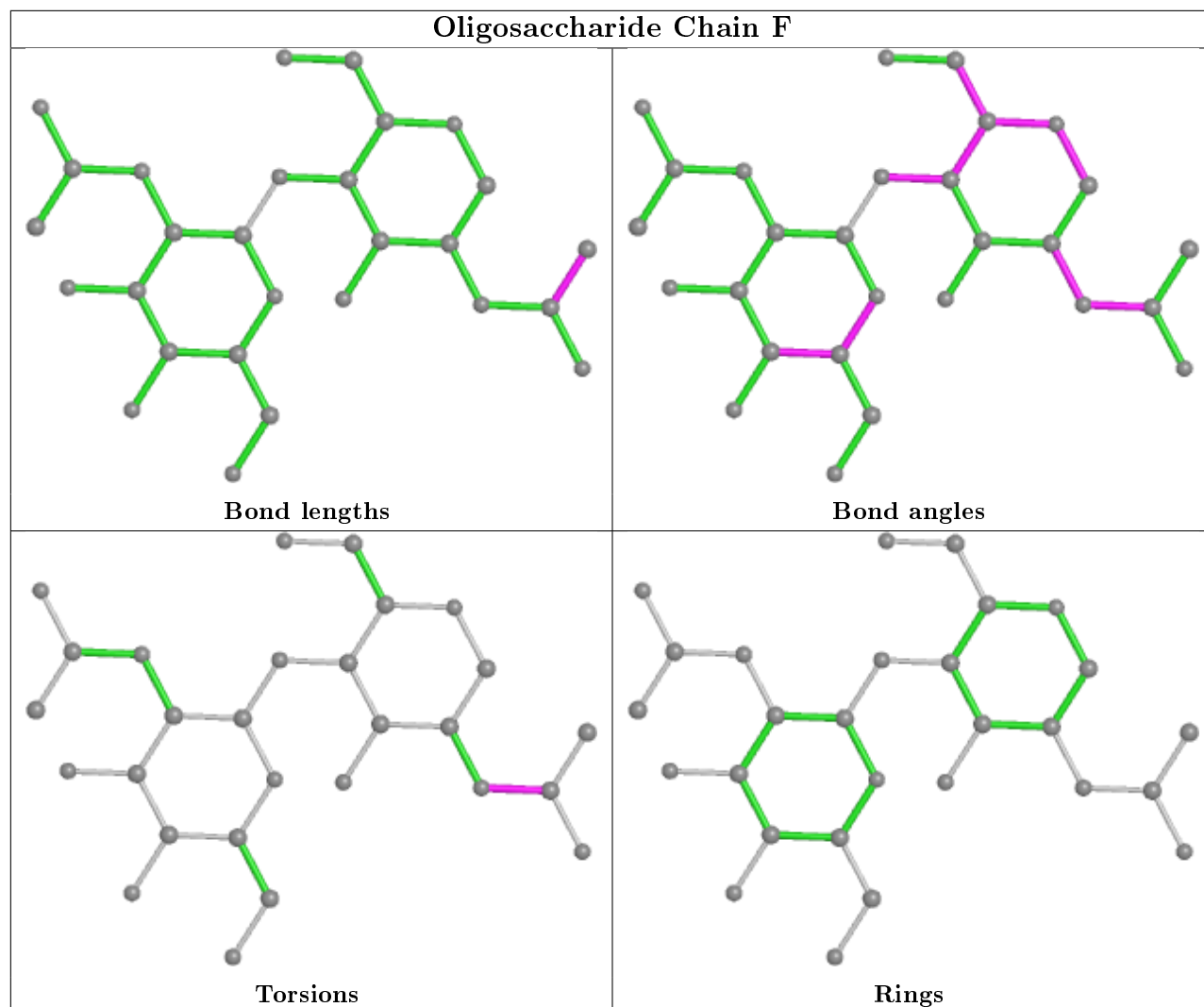
There are no ring outliers.

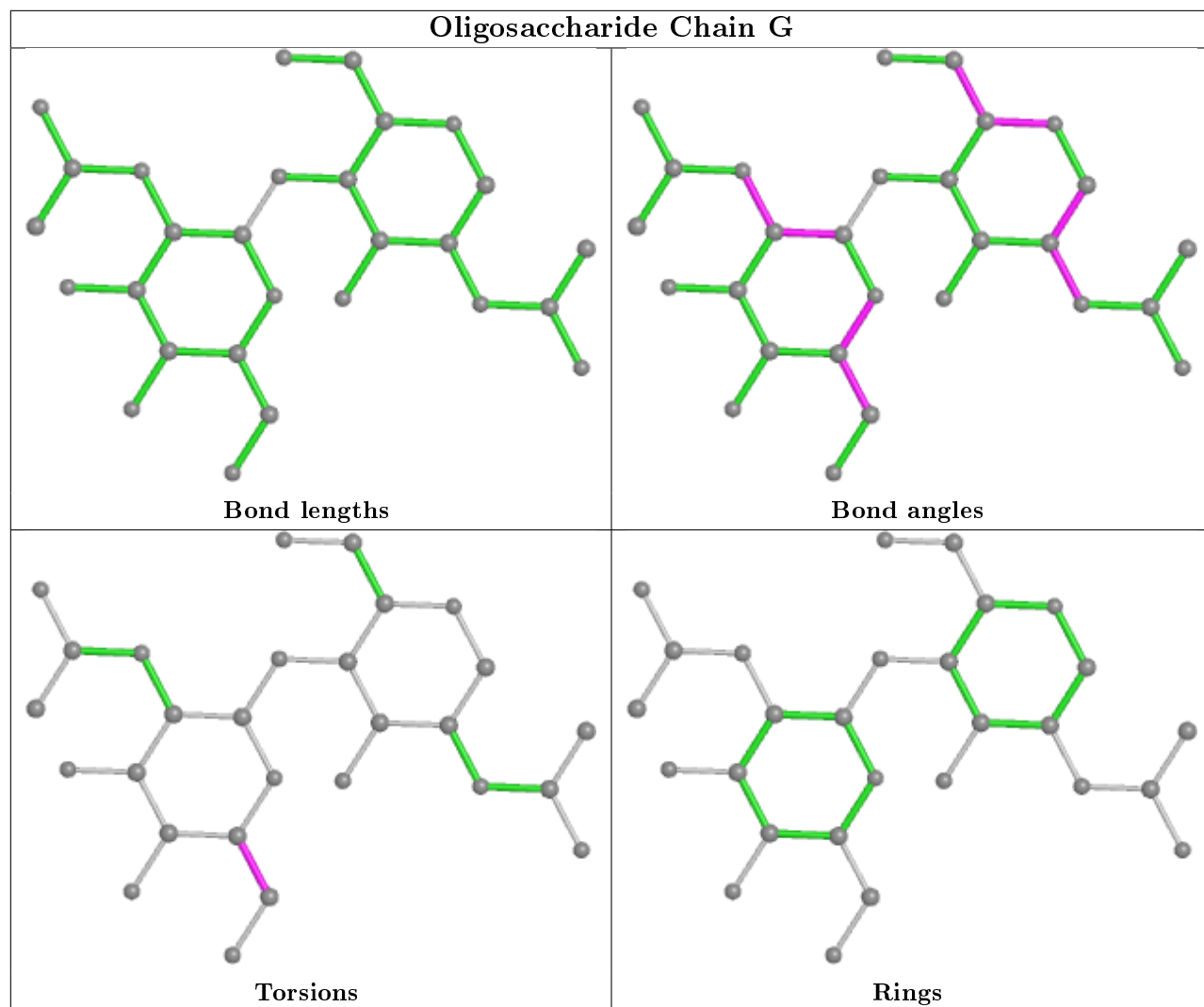
No monomer is involved in short contacts.

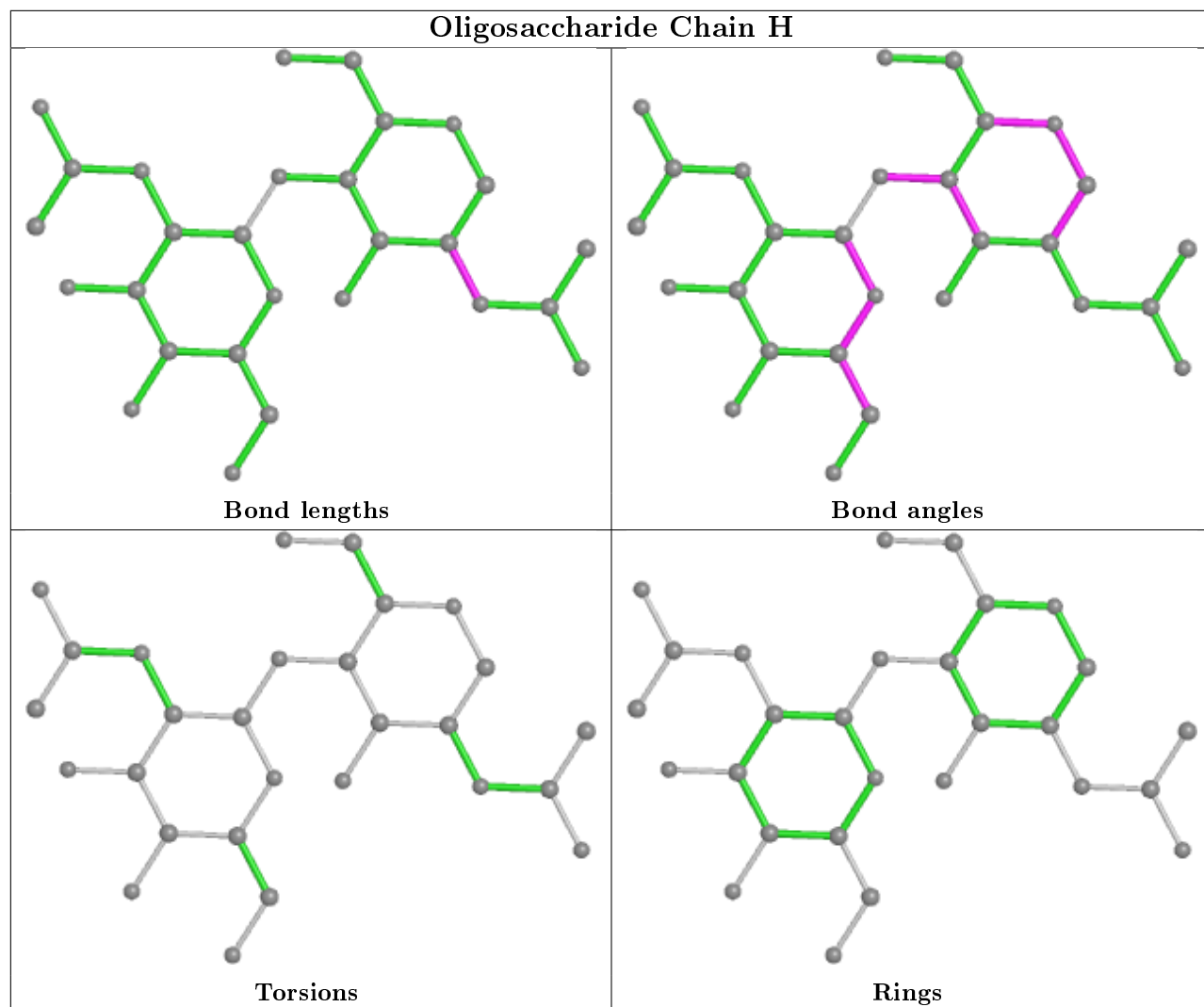
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

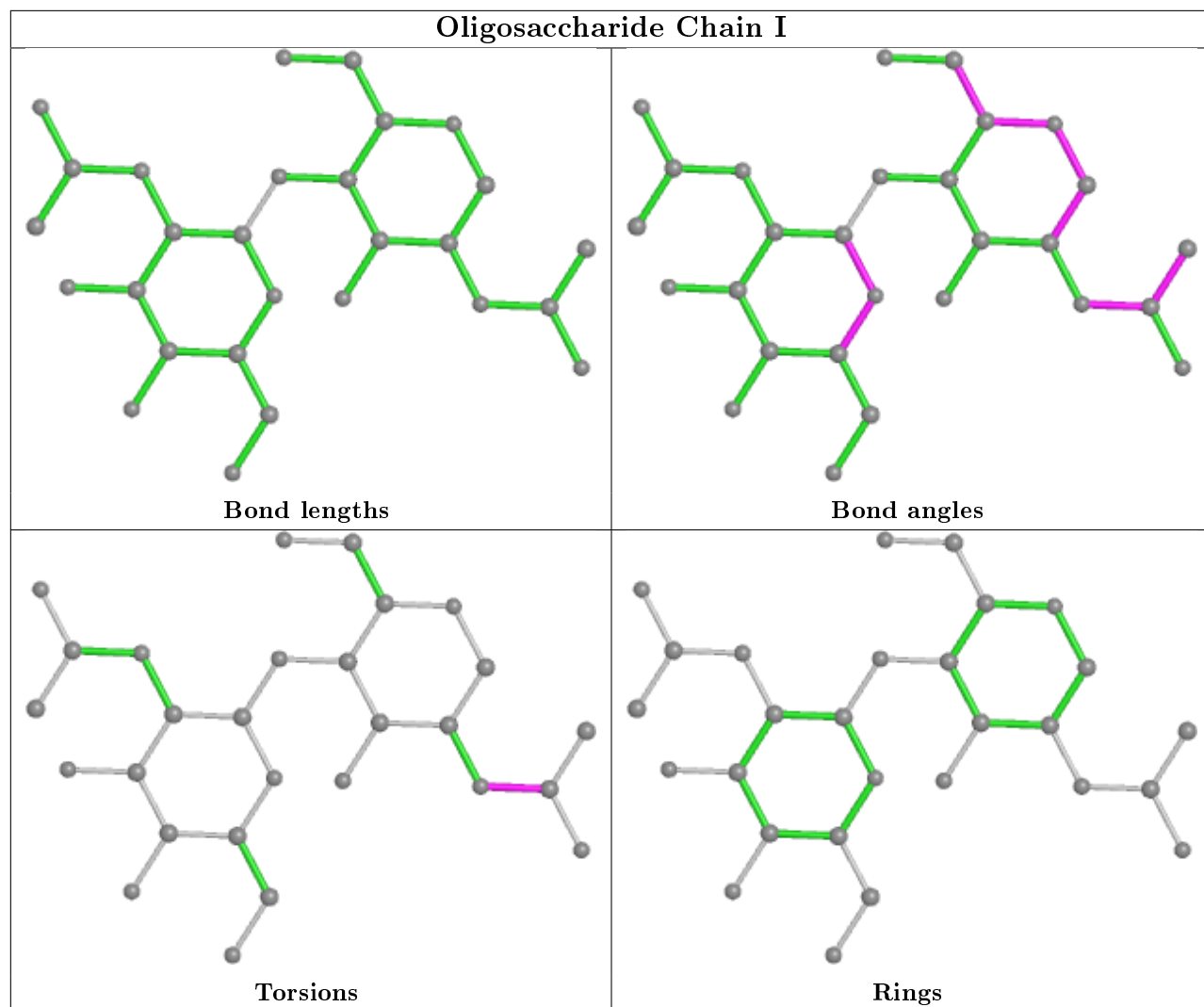


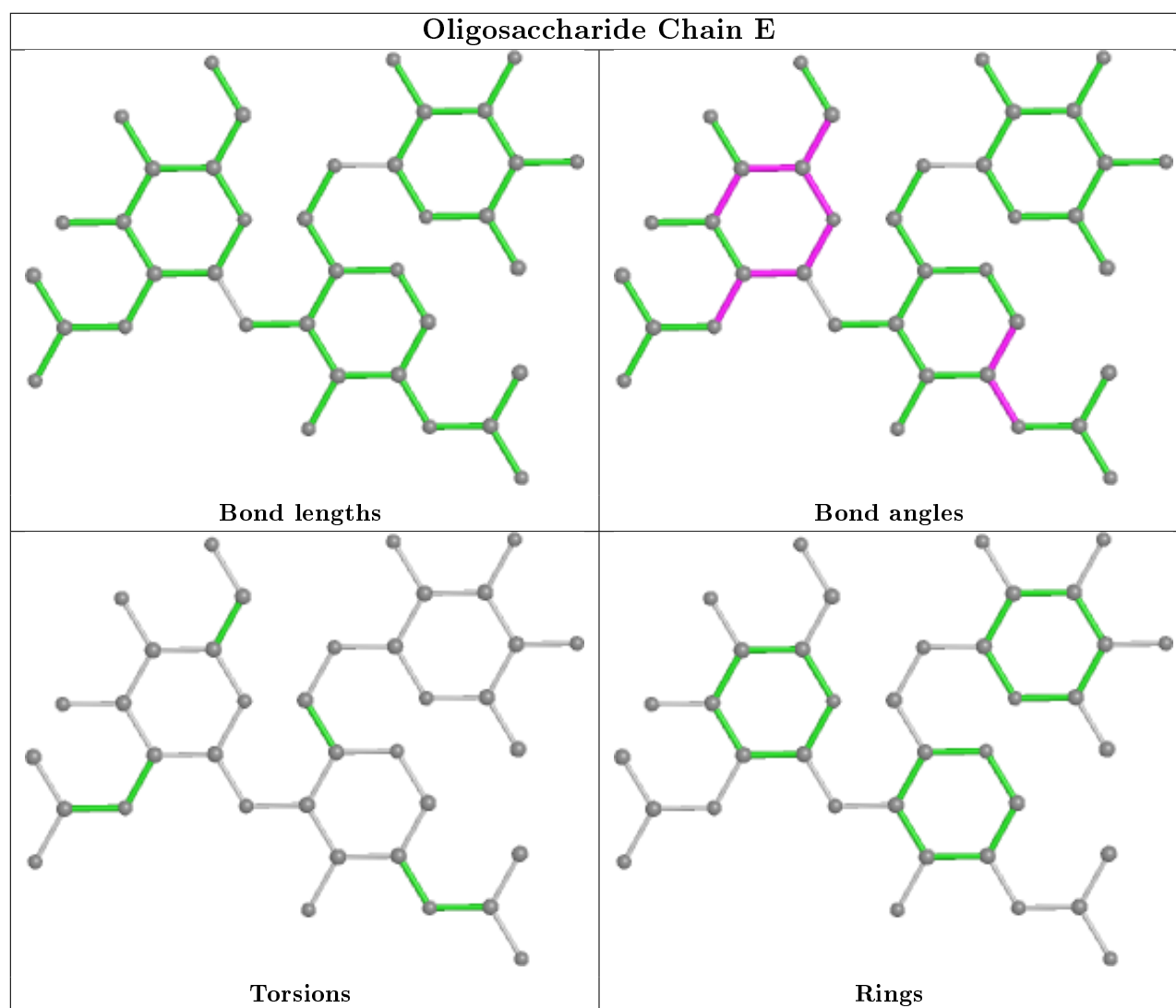












## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	B	407	1	14,14,15	1.00	1 (7%)	17,19,21	1.79	4 (23%)
4	CTP	A	410	-	23,30,30	1.25	2 (8%)	30,47,47	1.40	3 (10%)
4	CTP	B	408	-	23,30,30	0.87	0	30,47,47	1.93	7 (23%)



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
5	NAG	B	407	1	-	1/6/23/26	0/1/1/1
4	CTP	A	410	-	-	2/20/38/38	0/2/2/2
4	CTP	B	408	-	-	2/20/38/38	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	410	CTP	O4'-C1'	4.05	1.46	1.41
4	A	410	CTP	C2'-C1'	-2.27	1.50	1.53
5	B	407	NAG	C1-C2	2.08	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	408	CTP	PB-O3A-PA	-5.62	113.53	132.83
4	B	408	CTP	C2-N3-C4	5.09	121.50	116.34
5	B	407	NAG	O5-C1-C2	-4.40	104.35	111.29
4	A	410	CTP	PB-O3A-PA	-3.89	119.47	132.83
5	B	407	NAG	O5-C5-C6	3.57	112.80	107.20
4	A	410	CTP	C2-N3-C4	3.41	119.79	116.34
4	A	410	CTP	O2B-PB-O1B	3.19	128.00	112.24
4	B	408	CTP	PB-O3B-PG	-2.88	122.93	132.83
5	B	407	NAG	C4-C3-C2	-2.88	106.80	111.02
4	B	408	CTP	N4-C4-N3	2.73	120.81	116.49
4	B	408	CTP	O4'-C1'-C2'	2.19	110.13	106.93
4	B	408	CTP	O3G-PG-O1G	2.16	119.14	110.68
5	B	407	NAG	C1-C2-N2	2.12	114.11	110.49
4	B	408	CTP	O3G-PG-O2G	2.09	115.61	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	410	CTP	PB-O3A-PA-O2A
5	B	407	NAG	C3-C2-N2-C7
4	B	408	CTP	PG-O3B-PB-O3A
4	A	410	CTP	PG-O3B-PB-O1B

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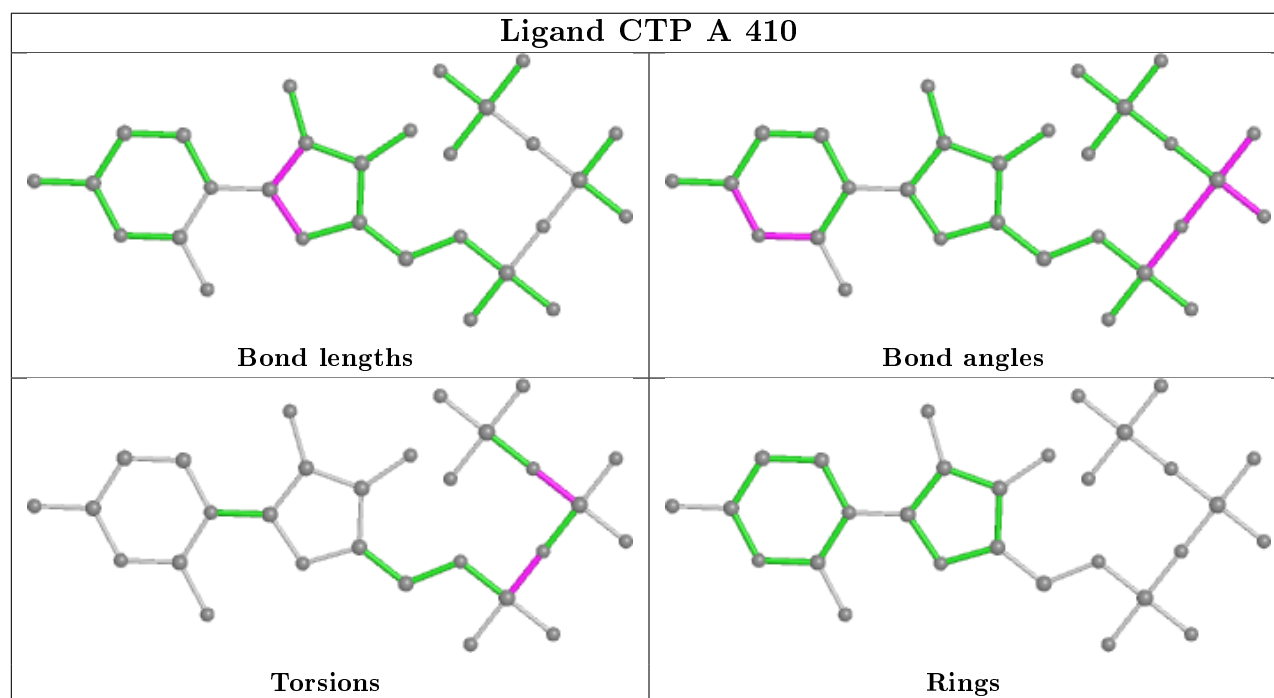
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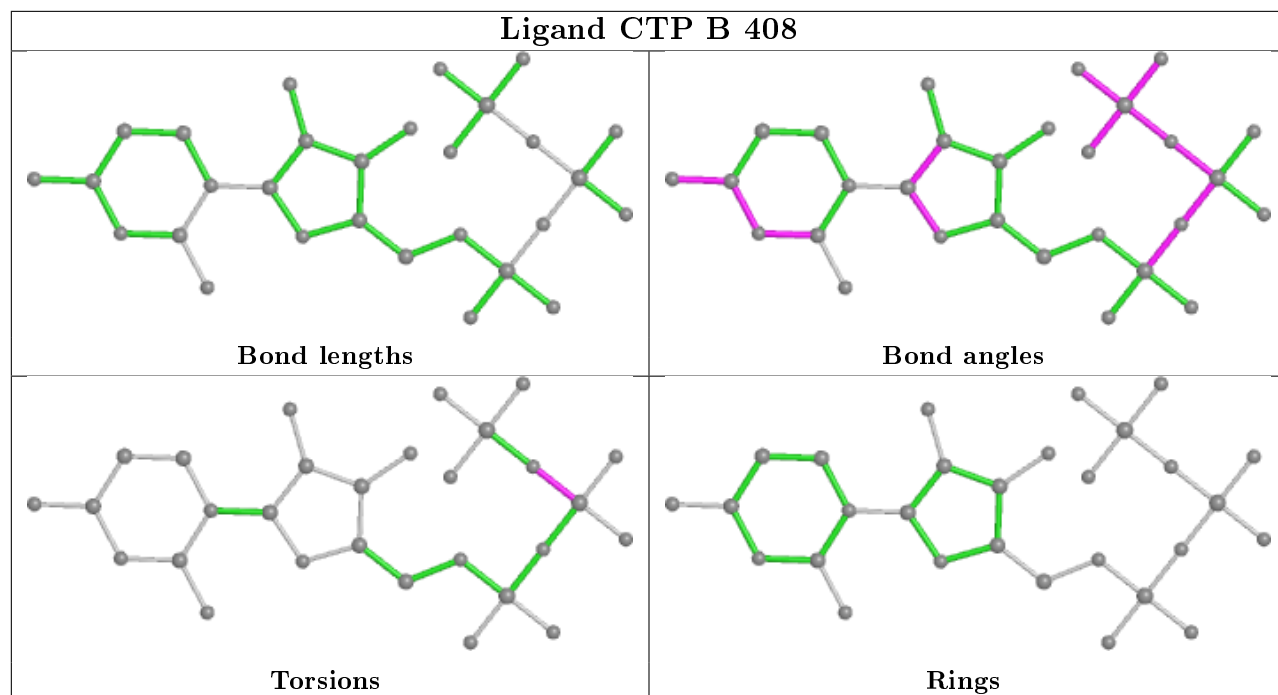
Mol	Chain	Res	Type	Atoms
4	B	408	CTP	PG-O3B-PB-O1B

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	290/323 (89%)	-0.19	7 (2%) 59 57	20, 29, 51, 74	0
1	B	279/323 (86%)	0.03	13 (4%) 31 30	22, 36, 62, 100	0
All	All	569/646 (88%)	-0.08	20 (3%) 44 41	20, 32, 56, 100	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	LYS	6.7
1	B	293	HIS	4.4
1	B	295	SER	4.1
1	B	291	ASN	4.0
1	B	296	PRO	3.9
1	A	353	SER	3.9
1	A	380	ALA	3.2
1	A	348	THR	3.1
1	B	355	GLN	2.9
1	A	352	GLU	2.9
1	B	287	ARG	2.7
1	A	293	HIS	2.7
1	B	88	SER	2.4
1	B	380	ALA	2.4
1	B	195	GLU	2.3
1	A	295	SER	2.1
1	B	290	LYS	2.1
1	B	134	HIS	2.1
1	A	355	GLN	2.0
1	B	298	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

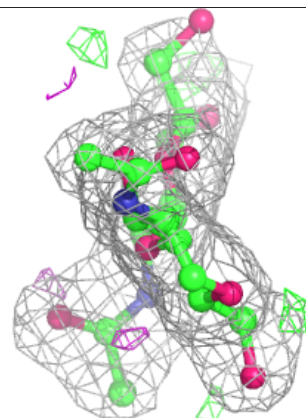
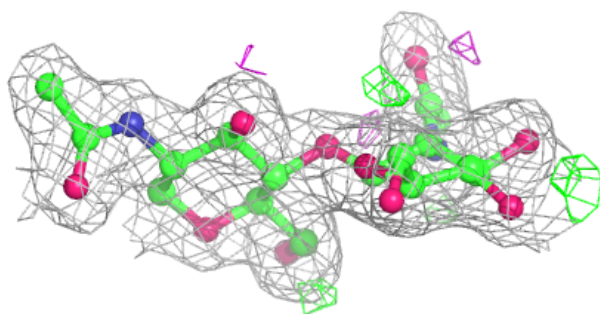
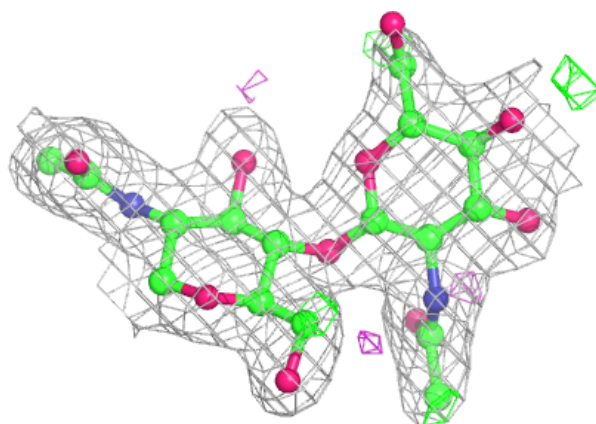
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	I	2	14/15	0.84	0.38	68,80,86,90	0
2	NAG	D	1	14/15	0.87	0.26	41,53,61,67	0
2	NAG	I	1	14/15	0.90	0.18	48,57,67,69	0
2	NAG	G	2	14/15	0.91	0.14	36,45,56,64	0
2	NAG	F	2	14/15	0.91	0.12	40,45,62,64	0
2	NAG	H	2	14/15	0.92	0.26	51,56,64,72	0
2	NAG	D	2	14/15	0.92	0.35	65,72,82,83	0
2	NAG	F	1	14/15	0.92	0.12	24,30,37,38	0
2	NAG	C	2	14/15	0.93	0.09	41,49,59,67	0
3	NAG	E	1	14/15	0.93	0.08	24,27,31,37	0
3	NAG	E	2	14/15	0.94	0.11	37,43,62,63	0
2	NAG	C	1	14/15	0.95	0.08	28,31,37,45	0
2	NAG	H	1	14/15	0.96	0.07	31,37,41,43	0
2	NAG	G	1	14/15	0.97	0.07	26,29,32,36	0
3	FUC	E	3	10/11	0.97	0.08	33,36,40,41	0

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

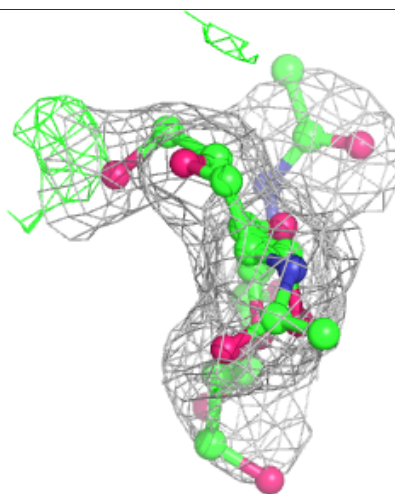
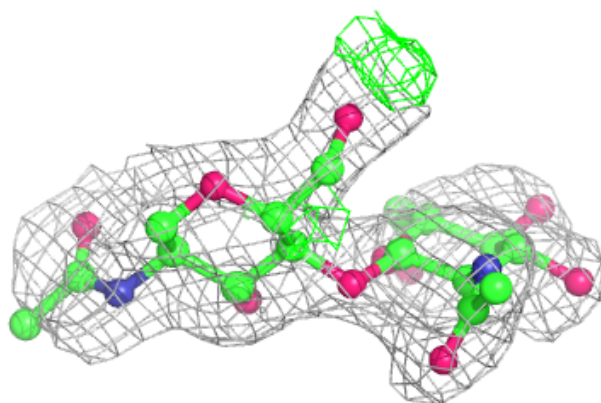
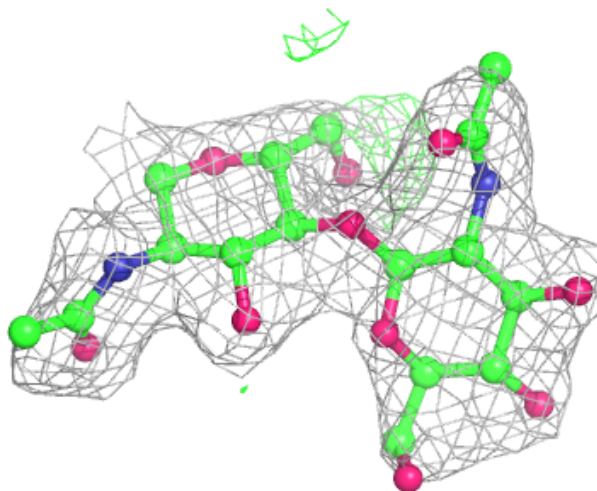
**Electron density around Chain C:**

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



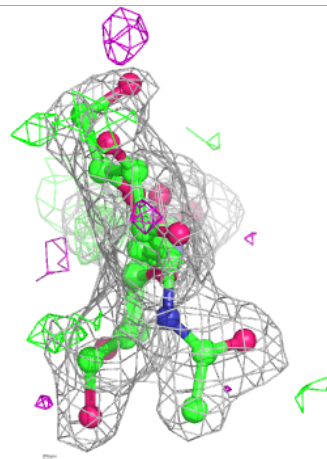
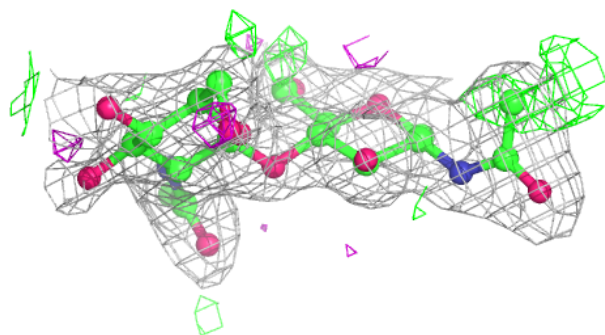
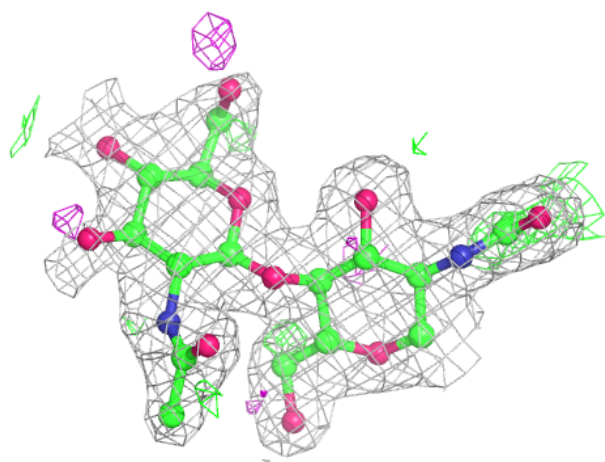
**Electron density around Chain D:**

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



**Electron density around Chain F:**

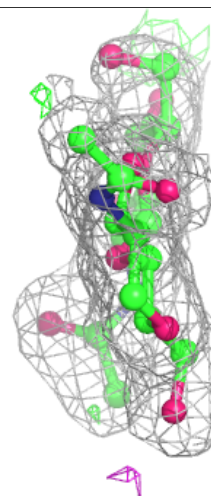
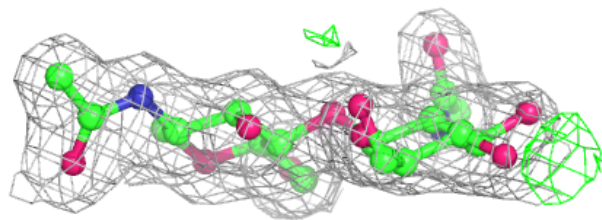
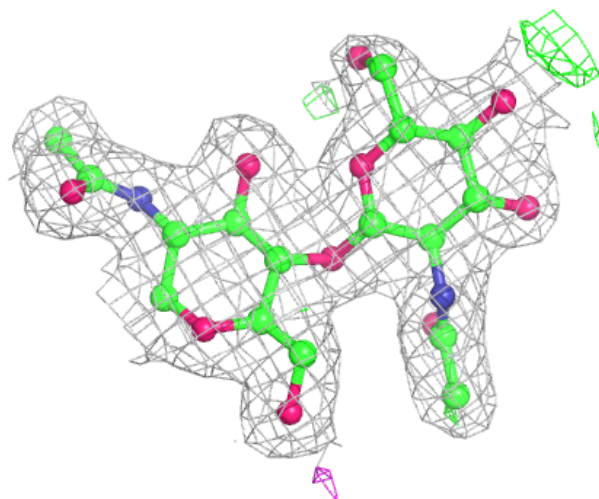
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





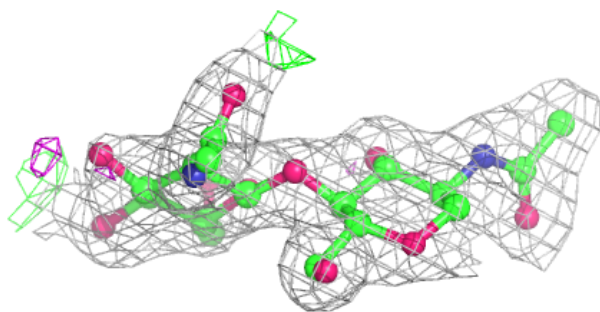
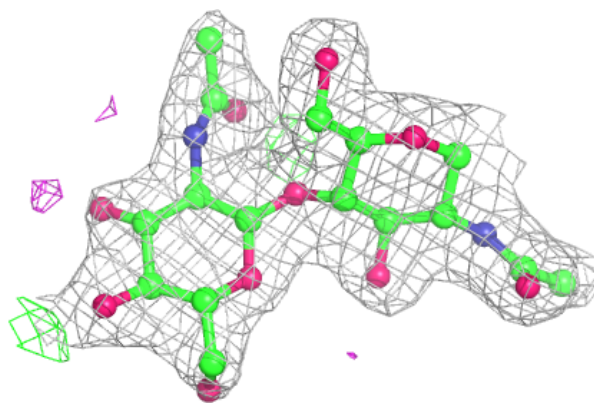
**Electron density around Chain G:**

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

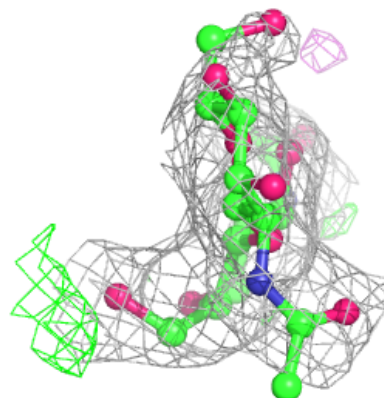
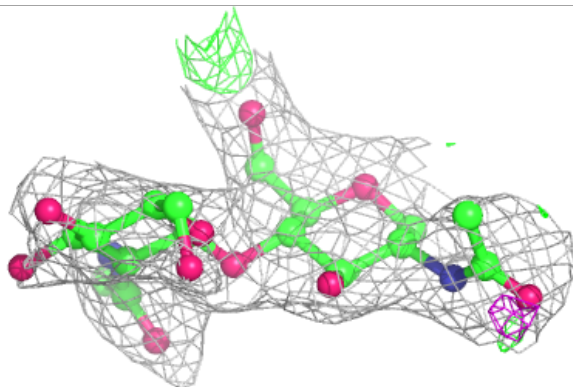
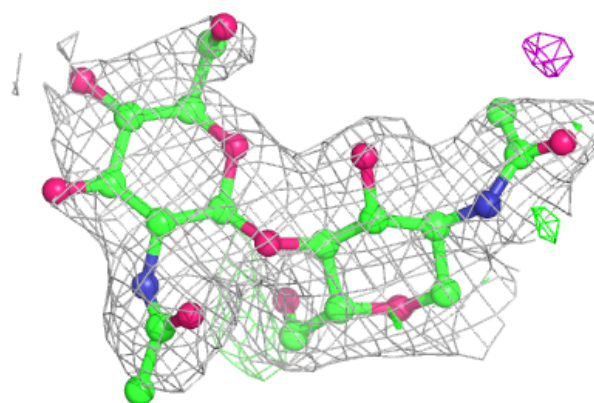


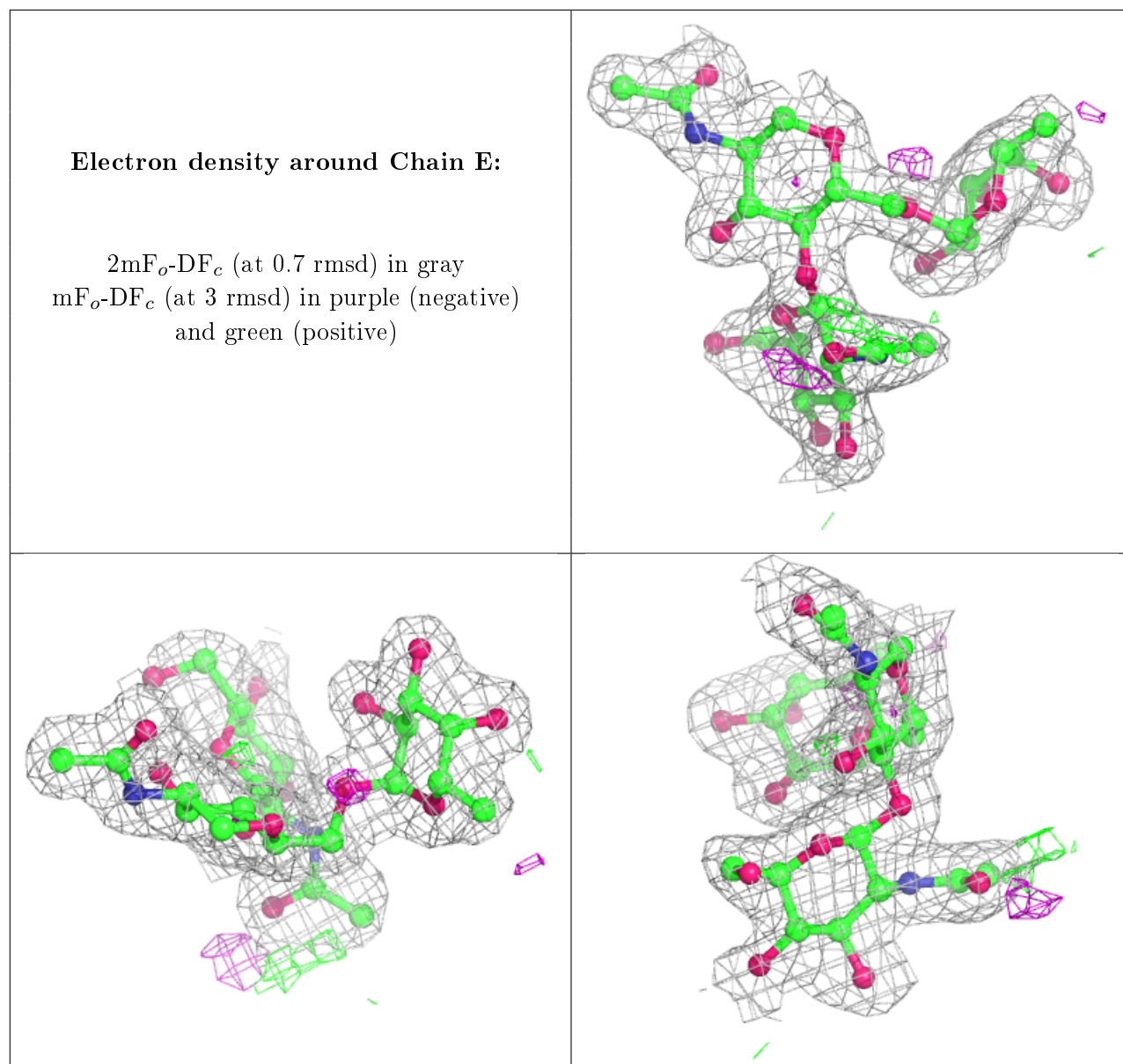
**Electron density around Chain H:**

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

**Electron density around Chain 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, 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.

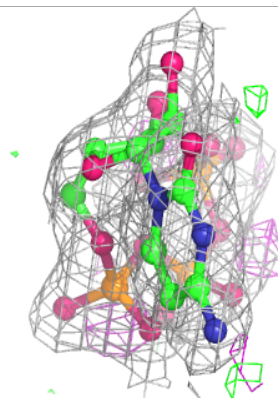
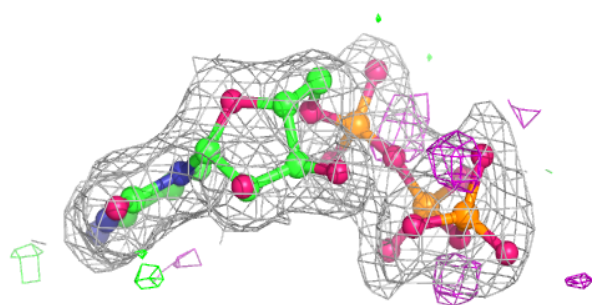
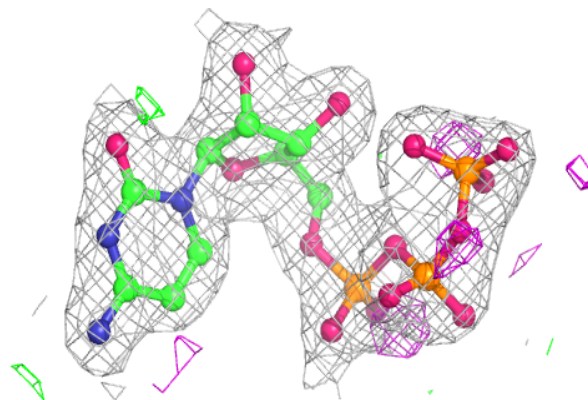
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	407	14/15	0.68	0.37	60,77,91,92	0
4	CTP	B	408	29/29	0.94	0.09	35,39,70,71	0
4	CTP	A	410	29/29	0.98	0.06	22,23,37,41	0

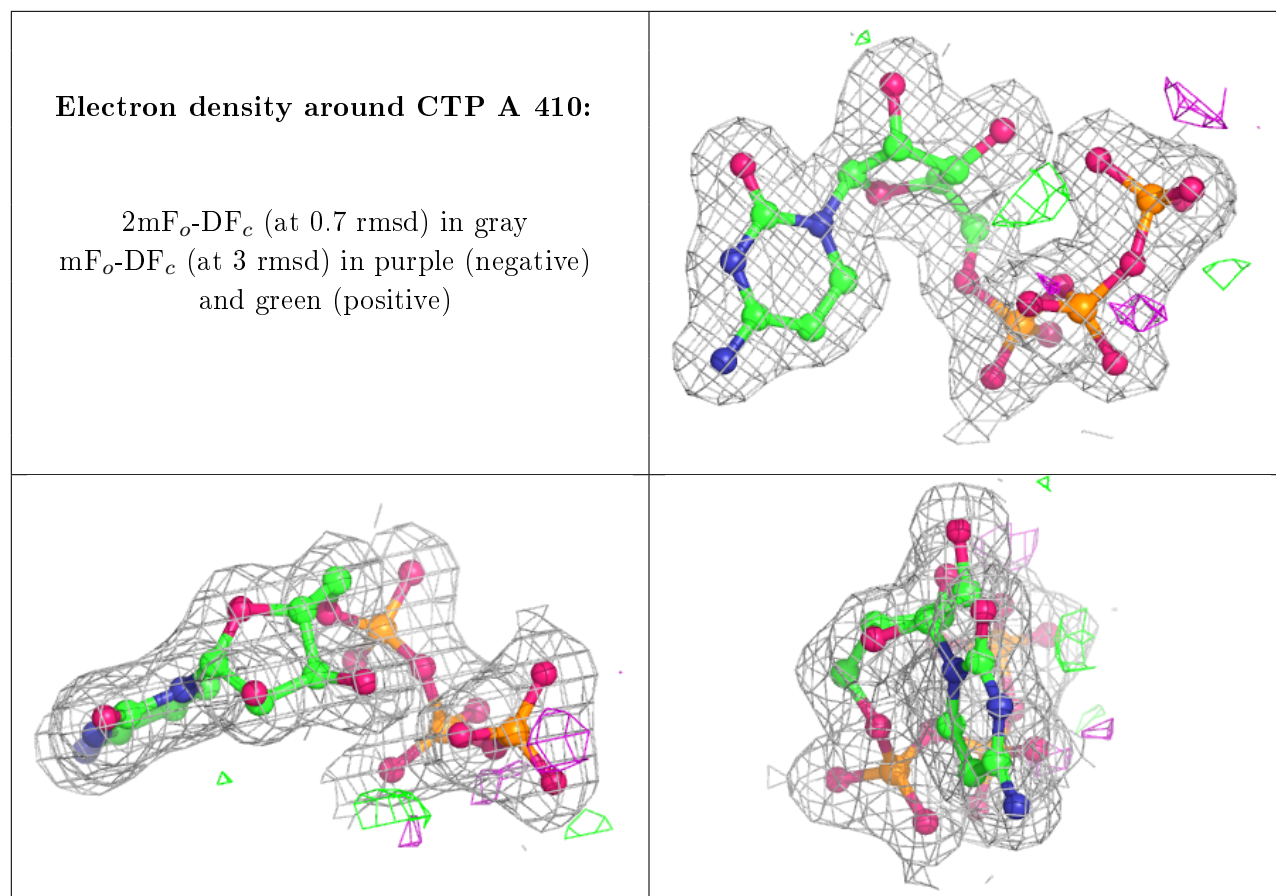
The following is a graphical depiction of the model fit to experimental electron density of all

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

**Electron density around CTP B 408:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.