



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2024 – 12:08 PM EDT

PDB ID : 4DW5  
Title : Crystal structure of the glycoprotein Erns from the pestivirus BVDV-1 in complex with a non-cleavable CpU dinucleotide  
Authors : Krey, T.; Bontems, F.; Vonnrhein, C.; Vaney, M.-C.; Bricogne, G.; Ruemenapf, T.; Rey, F.A.  
Deposited on : 2012-02-24  
Resolution : 2.21 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

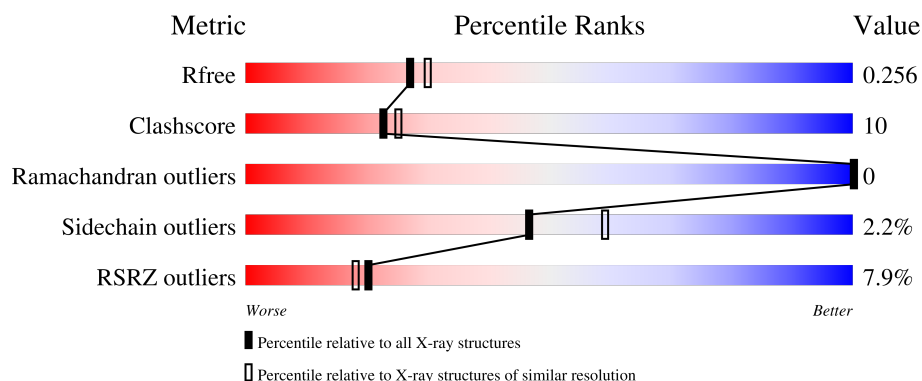
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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.



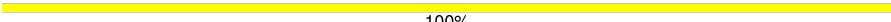
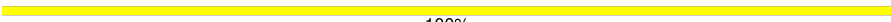

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7167 (2.24-2.20)
Clashscore	180529	8096 (2.24-2.20)
Ramachandran outliers	177936	8010 (2.24-2.20)
Sidechain outliers	177891	8011 (2.24-2.20)
RSRZ outliers	164620	7166 (2.24-2.20)

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	167	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>5%</div> </div> </div>
1	B	167	<div> <div>10%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
2	C	6	<div> <div></div> <div>100%</div> </div>
3	D	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	2	 100%
3	G	2	 100%
4	F	7	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	U5P	B	207	-	X	-	-
6	SO4	A	206	-	X	-	-
9	1PE	A	209	-	X	X	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 3234 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.

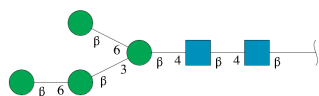
- Molecule 1 is a protein called E(rns) glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	9	0
			1291	804	230	237	20			
1	B	160	Total	C	N	O	S	1	9	0
			1306	812	233	241	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	expression tag	UNP Q96662
A	2	SER	-	expression tag	UNP Q96662
B	1	ARG	-	expression tag	UNP Q96662
B	2	SER	-	expression tag	UNP Q96662

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-3)-[beta-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.



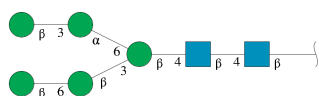
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



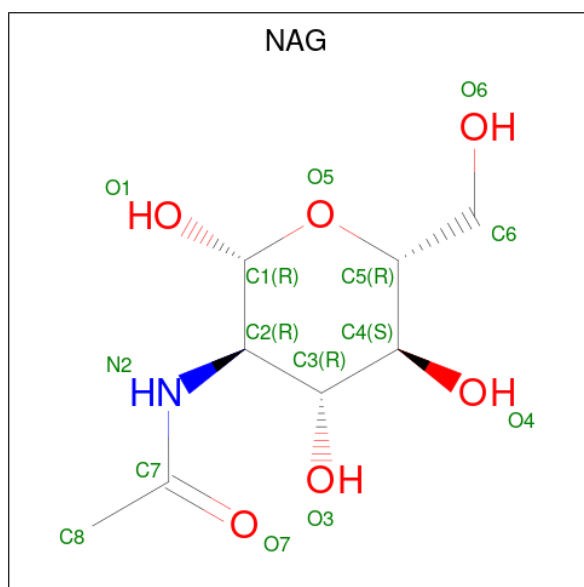
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	1	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-3)-[beta-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
4	F	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



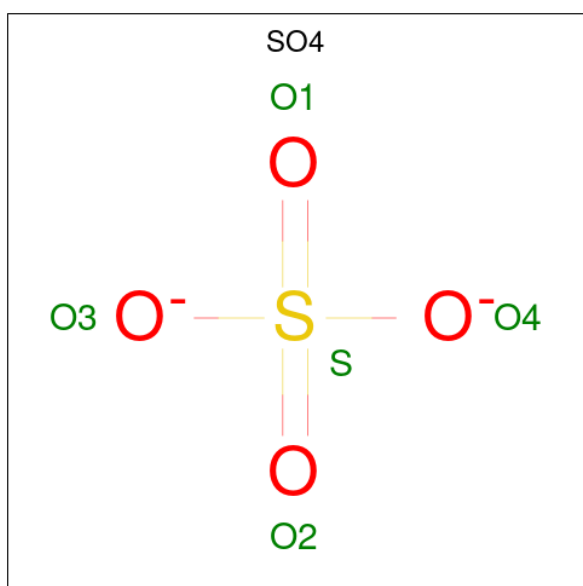
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



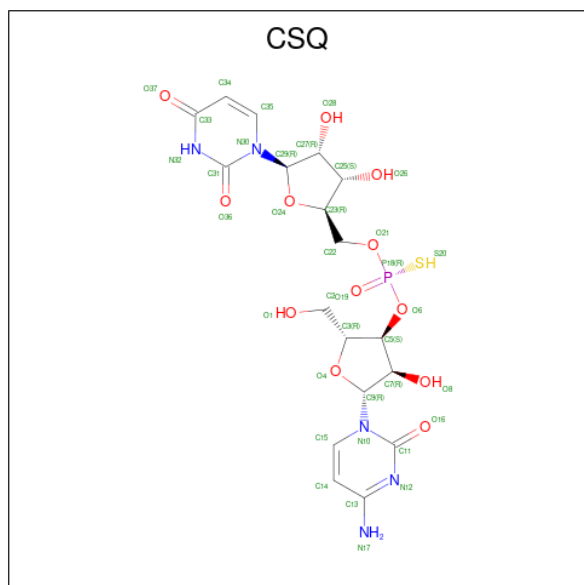
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O S	0	0
			5	4 1		
6	A	1	Total	O S	0	0
			5	4 1		
6	A	1	Total	O S	0	0
			5	4 1		
6	B	1	Total	O S	0	0
			5	4 1		
6	B	1	Total	O S	0	0
			5	4 1		
6	B	1	Total	O S	0	0
			5	4 1		

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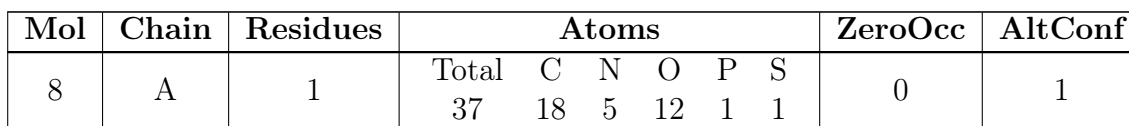
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is O-[(2R,3S,4R,5R)-5-(4-amino-2-oxypyrimidin-1(2H)-yl)-4-hydroxy-2-(hydroxymethyl)tetrahydrofuran-3-yl] O-{[(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl} hydrogen (R)-phosphorothioate (three-letter code: CSQ) (formula: C<sub>18</sub>H<sub>24</sub>N<sub>5</sub>O<sub>12</sub>PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	S	0	1
			37	18	5	12	1	1		

- Molecule 8 is O-[(2R,3S,4R,5R)-5-(4-amino-2-oxypyrimidin-1(2H)-yl)-4-hydroxy-2-(hydroxymethyl)tetrahydrofuran-3-yl] O-{[(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl} hydrogen (S)-phosphorothioate (three-letter code: CSV) (formula: C<sub>18</sub>H<sub>24</sub>N<sub>5</sub>O<sub>12</sub>PS).

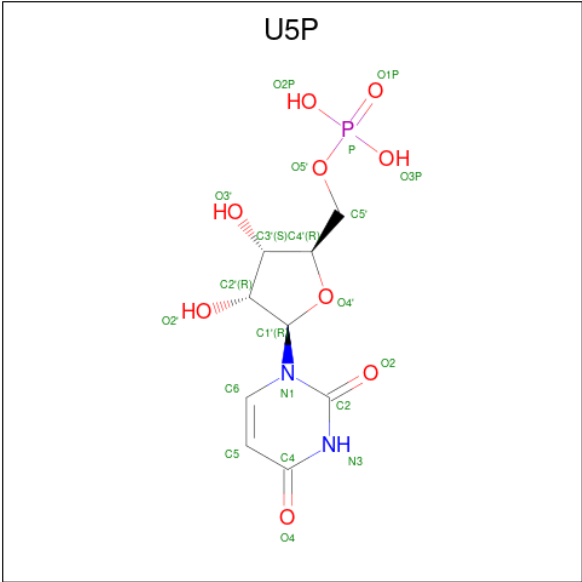


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- Chemical structure of 1PE (1,3,5,7-tetrahydroxyheptane) is shown. The structure is a zigzag line representing the carbon chain, with hydroxyl groups (OH) attached to carbons 1, 3, 5, and 7. The carbons are labeled C12, C22, C23, C13, C24, C14, C25, C15, C26, and C16. The hydroxyl groups are labeled OH12, OH13, OH14, and OH17.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	1	0
			16	10	6		

- 





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			9	5	2	2		


- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	103	Total	O	0	0
			103	103		
11	B	77	Total	O	0	0
			77	77		

### 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.

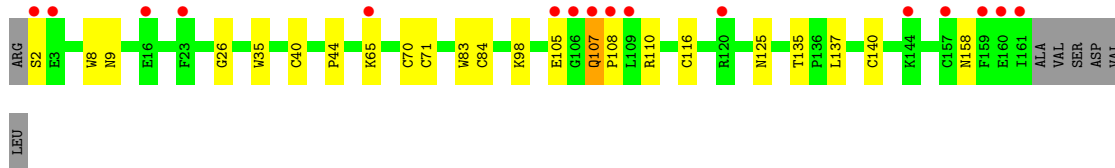
- Molecule 1: E(rns) glycoprotein

Chain A: 



- Molecule 1: E(rns) glycoprotein

Chain B: 

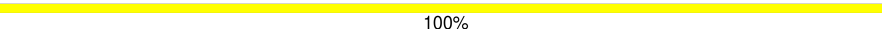


- Molecule 2: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 

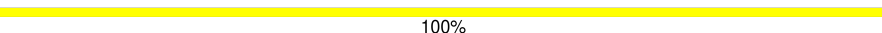


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 



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

Chain E: 

MAG1  
MAG2

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

Chain G:

100%

MAG1  
MAG2

- Molecule 4: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-3)-[beta-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 F:

100%

MAG1  
MAG2  
BM3  
BM4  
BM5  
MAG  
BM7

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.34Å 105.34Å 211.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.14 – 2.21 47.14 – 2.21	Depositor EDS
% Data completeness (in resolution range)	93.8 (47.14-2.21) 94.3 (47.14-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.22Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.2, BUSTER 2.9.2	Depositor
R, $R_{free}$	0.216 , 0.248 0.224 , 0.256	Depositor DCC
$R_{free}$ test set	1672 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 69.4	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	0.94	EDS
Total number of atoms	3234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, U5P, MAN, CSV, BMA, SO4, 1PE, CSQ

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	0.57	0/1347	0.72	1/1823 (0.1%)
1	B	0.52	0/1363	0.69	0/1847
All	All	0.55	0/2710	0.71	1/3670 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ARG	N-CA-C	-6.08	94.58	111.00

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	1291	0	1247	29	0
1	B	1306	0	1261	24	0
2	C	72	0	61	0	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
3	G	28	0	25	0	0
4	F	83	0	70	0	0
5	A	42	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	42	0	39	2	0
6	A	15	0	0	0	0
6	B	20	0	0	0	0
7	A	37	0	24	4	0
8	A	37	0	24	7	0
9	A	16	0	22	11	0
10	B	9	0	3	2	0
11	A	103	0	0	1	0
11	B	77	0	0	1	0
All	All	3234	0	2865	58	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 10.

The worst 5 of 58 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)
8:A:208[B]:CSV:S20	8:A:208[B]:CSV:P18	1.52	1.51
7:A:207[A]:CSQ:P18	7:A:207[A]:CSQ:S20	1.47	1.45
1:B:70[B]:CYS:SG	1:B:71[B]:CYS:HB3	1.60	1.40
1:B:116[B]:CYS:HB2	1:B:140[B]:CYS:SG	2.00	1.01
1:B:70[B]:CYS:SG	1:B:71[B]:CYS:CB	2.50	0.99

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	163/167 (98%)	157 (96%)	6 (4%)	0	100	100
1	B	167/167 (100%)	159 (95%)	8 (5%)	0	100	100
All	All	330/334 (99%)	316 (96%)	14 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	147/146 (101%)	146 (99%)	1 (1%)	81	89
1	B	149/146 (102%)	144 (97%)	5 (3%)	32	41
All	All	296/292 (101%)	290 (98%)	6 (2%)	47	63

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	105	GLU
1	B	107	GLN
1	B	110	ARG
1	B	2	SER
1	A	105	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	B	9	ASN
1	B	107	GLN

### 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 ⓘ

19 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	0.89	1 (7%)	17,19,21	2.52	7 (41%)
2	NAG	C	2	2	14,14,15	0.71	0	17,19,21	1.61	3 (17%)
2	BMA	C	3	2	11,11,12	0.83	0	15,15,17	1.33	2 (13%)
2	BMA	C	4	2	11,11,12	0.77	0	15,15,17	3.44	13 (86%)
2	BMA	C	5	2	11,11,12	0.86	0	15,15,17	2.15	6 (40%)
2	BMA	C	6	2	11,11,12	0.81	0	15,15,17	2.70	7 (46%)
3	NAG	D	1	3,1	14,14,15	0.99	1 (7%)	17,19,21	1.62	3 (17%)
3	NAG	D	2	3	14,14,15	1.00	1 (7%)	17,19,21	2.46	5 (29%)
3	NAG	E	1	3,1	14,14,15	0.97	1 (7%)	17,19,21	1.49	3 (17%)
3	NAG	E	2	3	14,14,15	1.03	1 (7%)	17,19,21	2.30	7 (41%)
4	NAG	F	1	1,4	14,14,15	0.88	1 (7%)	17,19,21	2.26	7 (41%)
4	NAG	F	2	4	14,14,15	0.81	0	17,19,21	1.54	4 (23%)
4	BMA	F	3	4	11,11,12	0.78	0	15,15,17	1.30	1 (6%)
4	BMA	F	4	4	11,11,12	0.79	0	15,15,17	3.41	11 (73%)
4	BMA	F	5	4	11,11,12	0.83	0	15,15,17	2.13	6 (40%)
4	MAN	F	6	4	11,11,12	0.76	0	15,15,17	1.39	1 (6%)
4	BMA	F	7	4	11,11,12	0.83	0	15,15,17	2.63	7 (46%)
3	NAG	G	1	3,1	14,14,15	1.07	1 (7%)	17,19,21	1.93	6 (35%)
3	NAG	G	2	3	14,14,15	1.00	1 (7%)	17,19,21	2.27	5 (29%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	BMA	C	4	2	-	2/2/19/22	0/1/1/1
2	BMA	C	5	2	-	2/2/19/22	1/1/1/1
2	BMA	C	6	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	BMA	F	4	4	-	2/2/19/22	0/1/1/1
4	BMA	F	5	4	-	2/2/19/22	1/1/1/1
4	MAN	F	6	4	-	2/2/19/22	0/1/1/1
4	BMA	F	7	4	-	2/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	C1-C2	2.76	1.56	1.52
3	G	2	NAG	C1-C2	2.71	1.56	1.52
3	D	1	NAG	C1-C2	2.67	1.56	1.52
3	G	1	NAG	C1-C2	2.61	1.55	1.52
3	E	1	NAG	C1-C2	2.61	1.55	1.52

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	7	BMA	C1-O5-C5	6.61	121.05	112.19
2	C	4	BMA	O2-C2-C1	6.35	123.77	109.22
4	F	4	BMA	O5-C1-C2	-6.25	95.87	110.79
2	C	4	BMA	O5-C1-C2	-6.22	95.96	110.79
2	C	1	NAG	C1-C2-N2	6.04	119.96	110.43

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

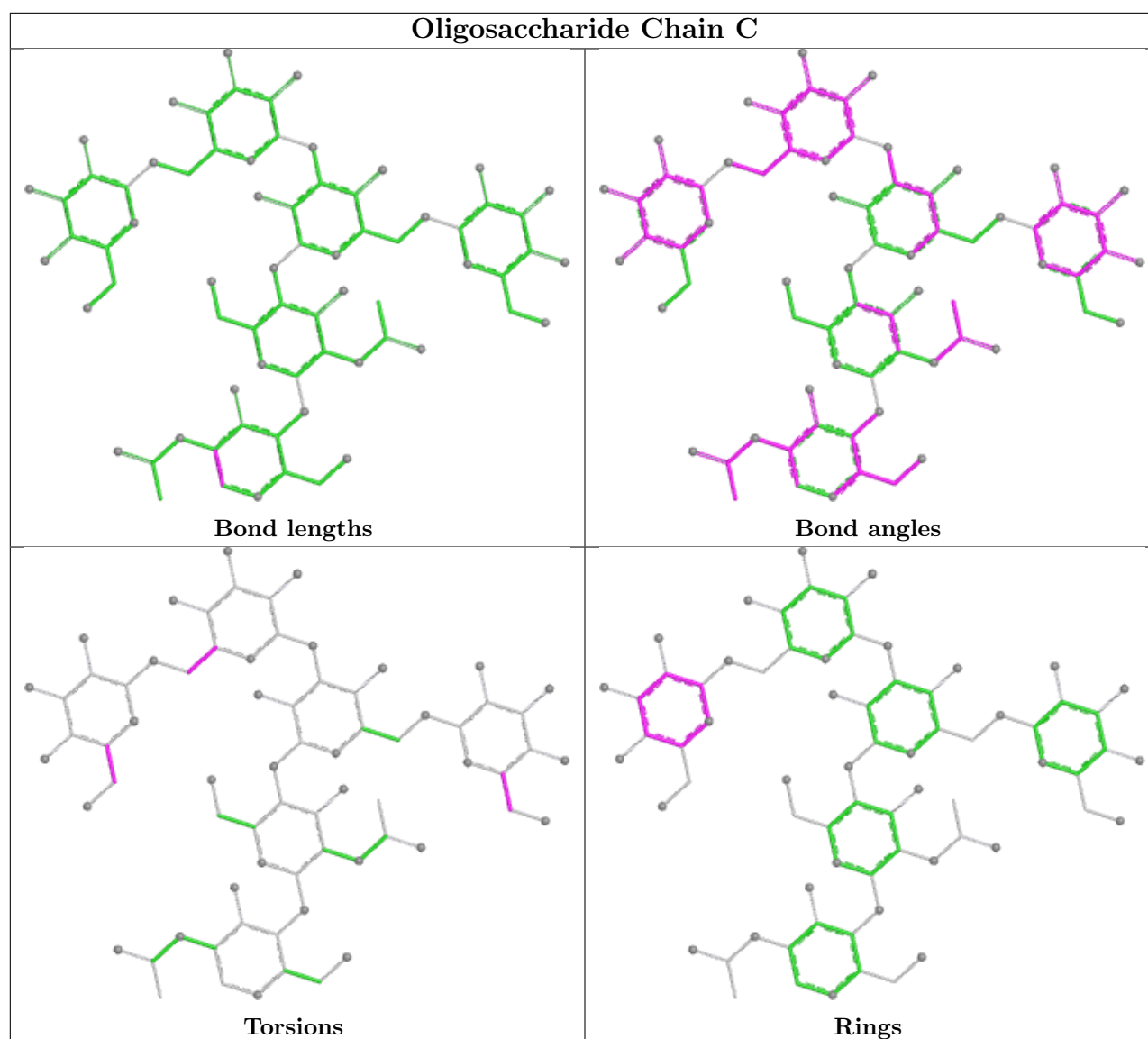
Mol	Chain	Res	Type	Atoms
4	F	7	BMA	C4-C5-C6-O6
4	F	5	BMA	O5-C5-C6-O6
2	C	5	BMA	O5-C5-C6-O6
2	C	5	BMA	C4-C5-C6-O6
4	F	5	BMA	C4-C5-C6-O6

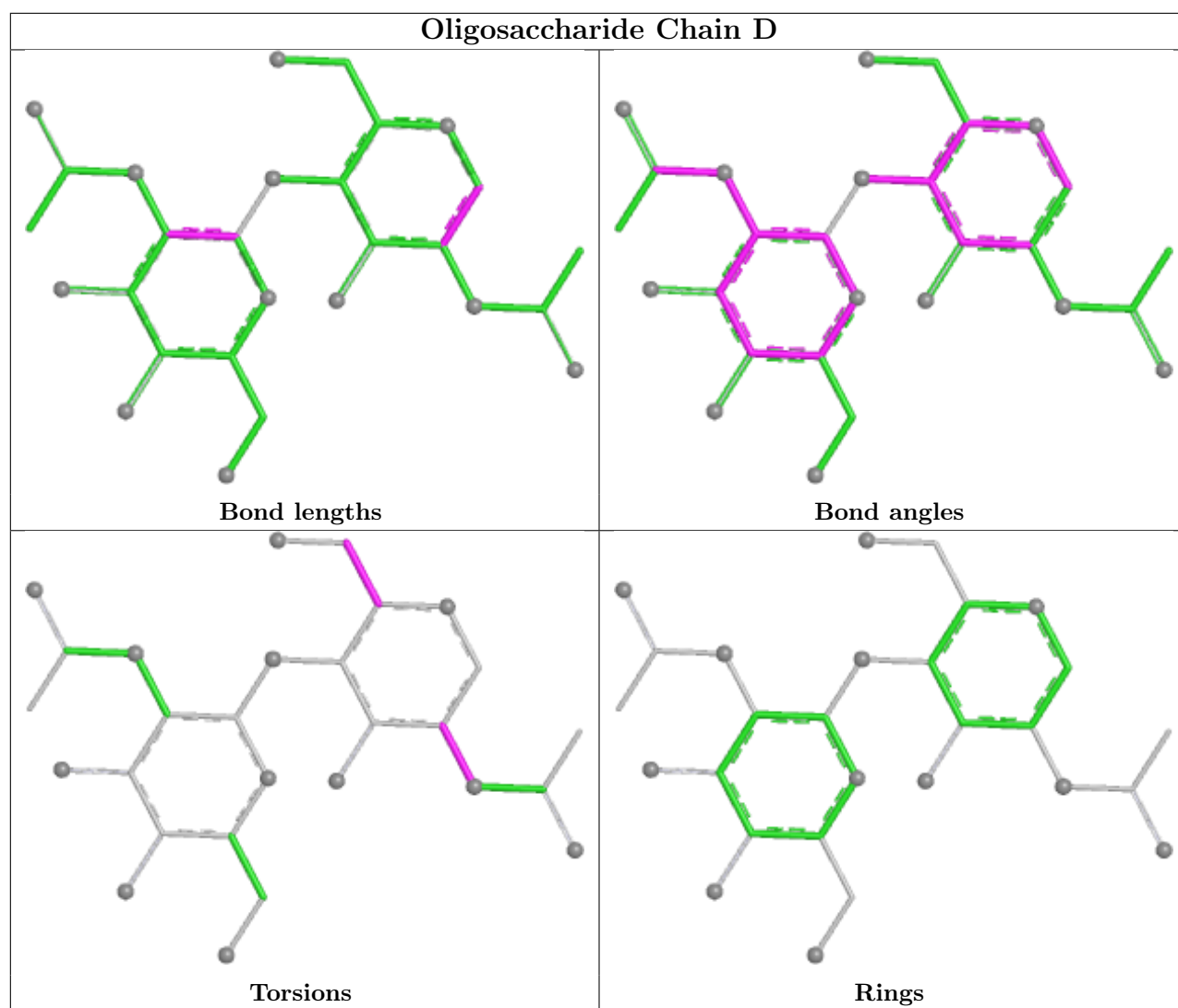
All (2) ring outliers are listed below:

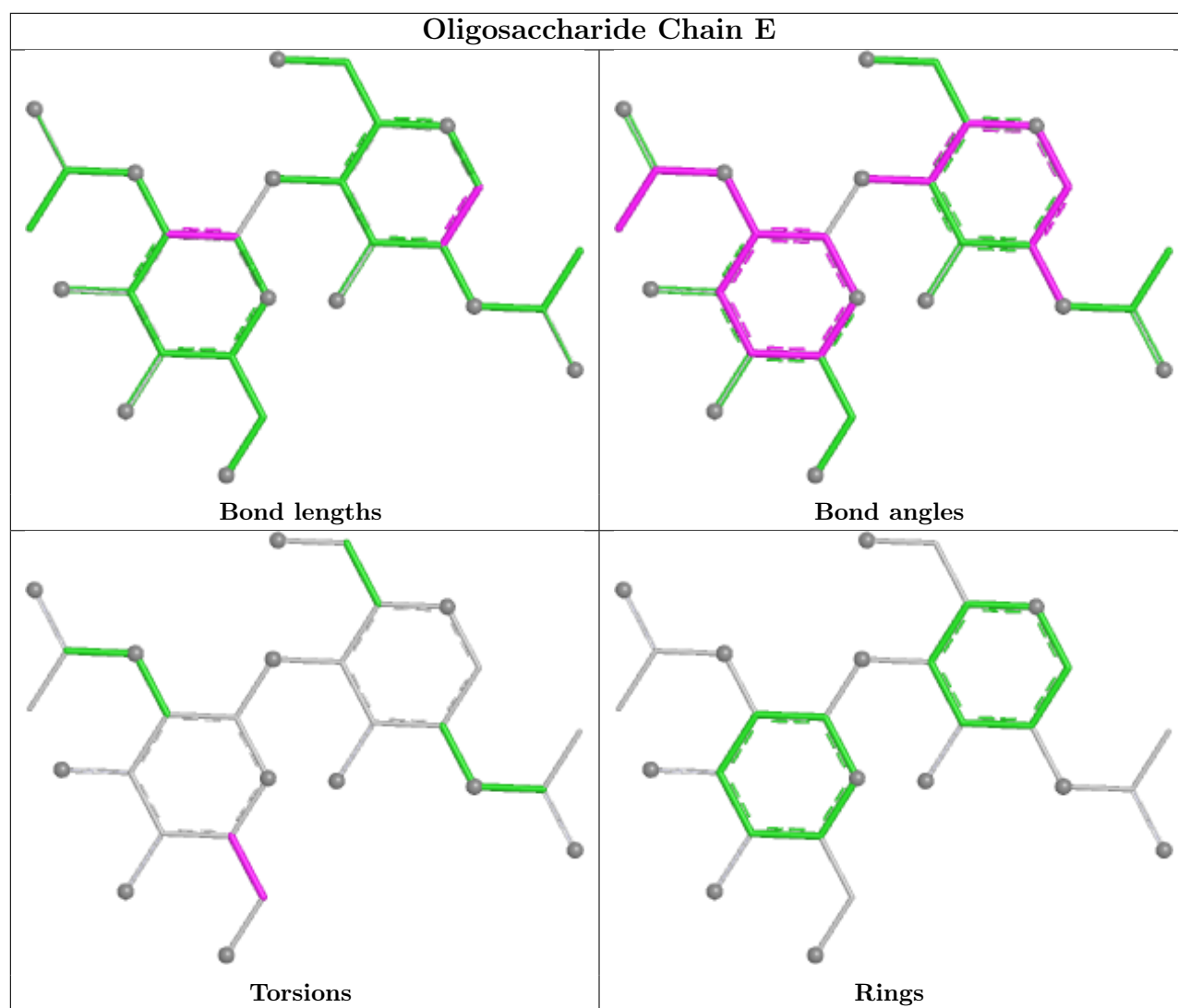
Mol	Chain	Res	Type	Atoms
2	C	5	BMA	C1-C2-C3-C4-C5-O5
4	F	5	BMA	C1-C2-C3-C4-C5-O5

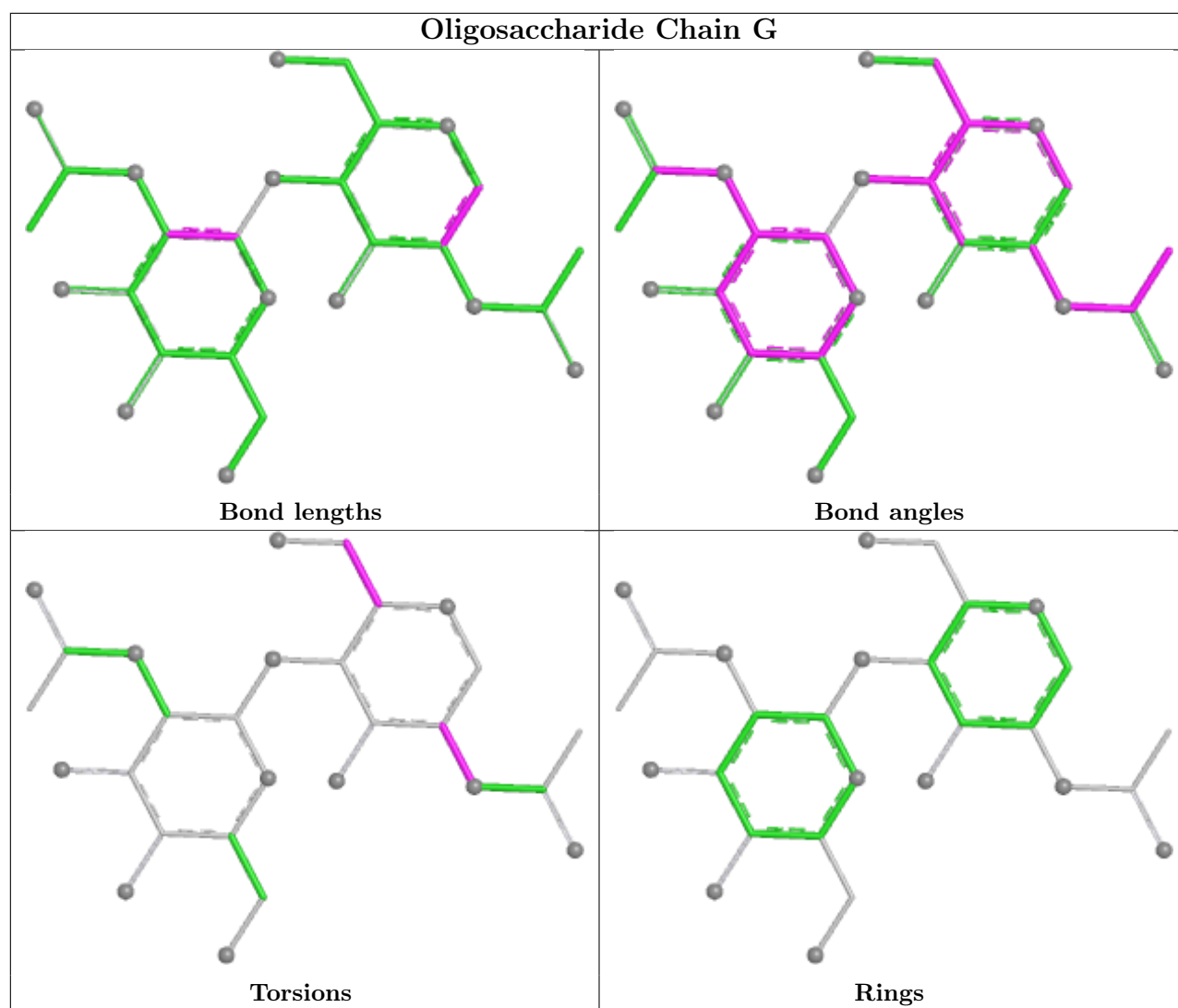
No monomer is involved in short contacts.

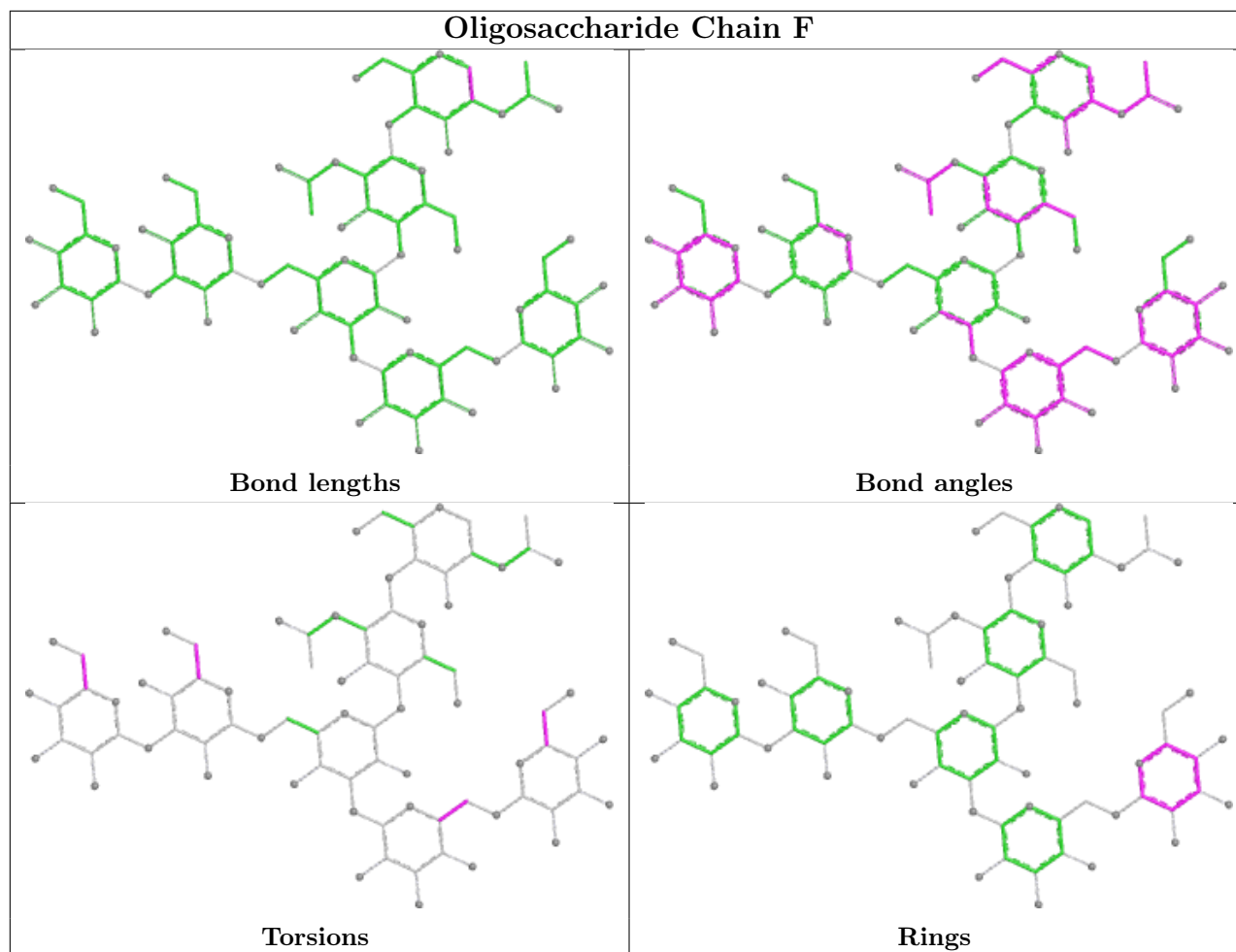
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

17 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
6	SO4	B	208	-	4,4,4	1.13	0	6,6,6	1.40	1 (16%)
5	NAG	A	201	1	14,14,15	1.01	1 (7%)	17,19,21	2.25	3 (17%)
5	NAG	B	201	1	14,14,15	0.98	1 (7%)	17,19,21	2.15	3 (17%)
7	CSQ	A	207[A]	-	37,40,40	1.01	2 (5%)	53,60,60	0.84	1 (1%)
6	SO4	A	205	-	4,4,4	0.46	0	6,6,6	1.79	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	B	204	-	4,4,4	1.11	0	6,6,6	1.37	1 (16%)
5	NAG	B	202	1	14,14,15	1.06	1 (7%)	17,19,21	1.94	6 (35%)
5	NAG	B	203	1	14,14,15	0.99	1 (7%)	17,19,21	1.54	4 (23%)
5	NAG	A	203	1	14,14,15	1.01	1 (7%)	17,19,21	2.11	4 (23%)
10	U5P	B	207	-	9,9,22	6.62	8 (88%)	12,12,33	7.09	10 (83%)
6	SO4	B	206	-	4,4,4	0.99	0	6,6,6	1.64	1 (16%)
8	CSV	A	208[B]	-	37,40,40	0.97	2 (5%)	53,60,60	0.79	1 (1%)
6	SO4	A	206	-	4,4,4	1.15	1 (25%)	6,6,6	2.17	3 (50%)
6	SO4	B	205	-	4,4,4	1.35	0	6,6,6	1.71	1 (16%)
6	SO4	A	204	-	4,4,4	0.67	0	6,6,6	0.98	0
9	1PE	A	209	-	15,15,15	1.32	2 (13%)	14,14,14	2.31	7 (50%)
5	NAG	A	202	1	14,14,15	1.02	1 (7%)	17,19,21	1.89	6 (35%)

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	A	201	1	-	0/6/23/26	0/1/1/1
5	NAG	B	201	1	-	0/6/23/26	0/1/1/1
7	CSQ	A	207[A]	-	-	3/19/53/53	0/4/4/4
5	NAG	B	202	1	-	2/6/23/26	0/1/1/1
5	NAG	B	203	1	-	0/6/23/26	0/1/1/1
5	NAG	A	203	1	-	2/6/23/26	0/1/1/1
10	U5P	B	207	-	-	-	0/1/1/2
8	CSV	A	208[B]	-	-	7/19/53/53	0/4/4/4
9	1PE	A	209	-	-	9/13/13/13	-
5	NAG	A	202	1	-	1/6/23/26	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	207	U5P	C2-N1	17.24	1.65	1.38
10	B	207	U5P	C1'-N1	4.30	1.55	1.46
10	B	207	U5P	C5-C4	4.14	1.52	1.43
10	B	207	U5P	O4-C4	-4.08	1.16	1.24
8	A	208[B]	CSV	C9-N10	3.81	1.58	1.47



The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	207	U5P	C1'-N1-C2	15.29	135.05	117.83
10	B	207	U5P	O2-C2-N1	13.21	136.13	122.78
10	B	207	U5P	O2-C2-N3	-9.01	104.89	121.49
5	A	203	NAG	C1-O5-C5	6.48	120.87	112.19
10	B	207	U5P	C1'-N1-C6	-6.24	108.68	120.41

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	209	1PE	C24-C14-OH5-C25
9	A	209	1PE	C25-C15-OH6-C26
9	A	209	1PE	C13-C23-OH3-C22
9	A	209	1PE	OH5-C14-C24-OH4
5	A	203	NAG	C4-C5-C6-O6

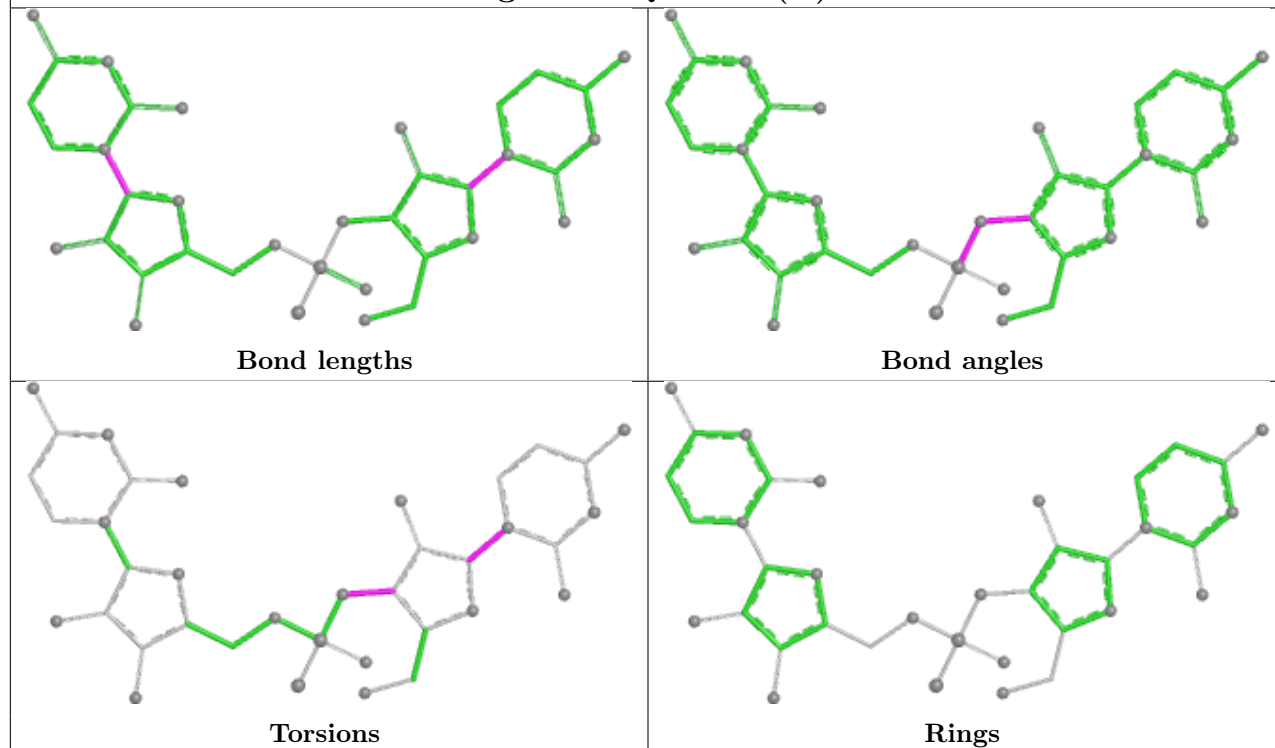
There are no ring outliers.

7 monomers are involved in 27 short contacts:

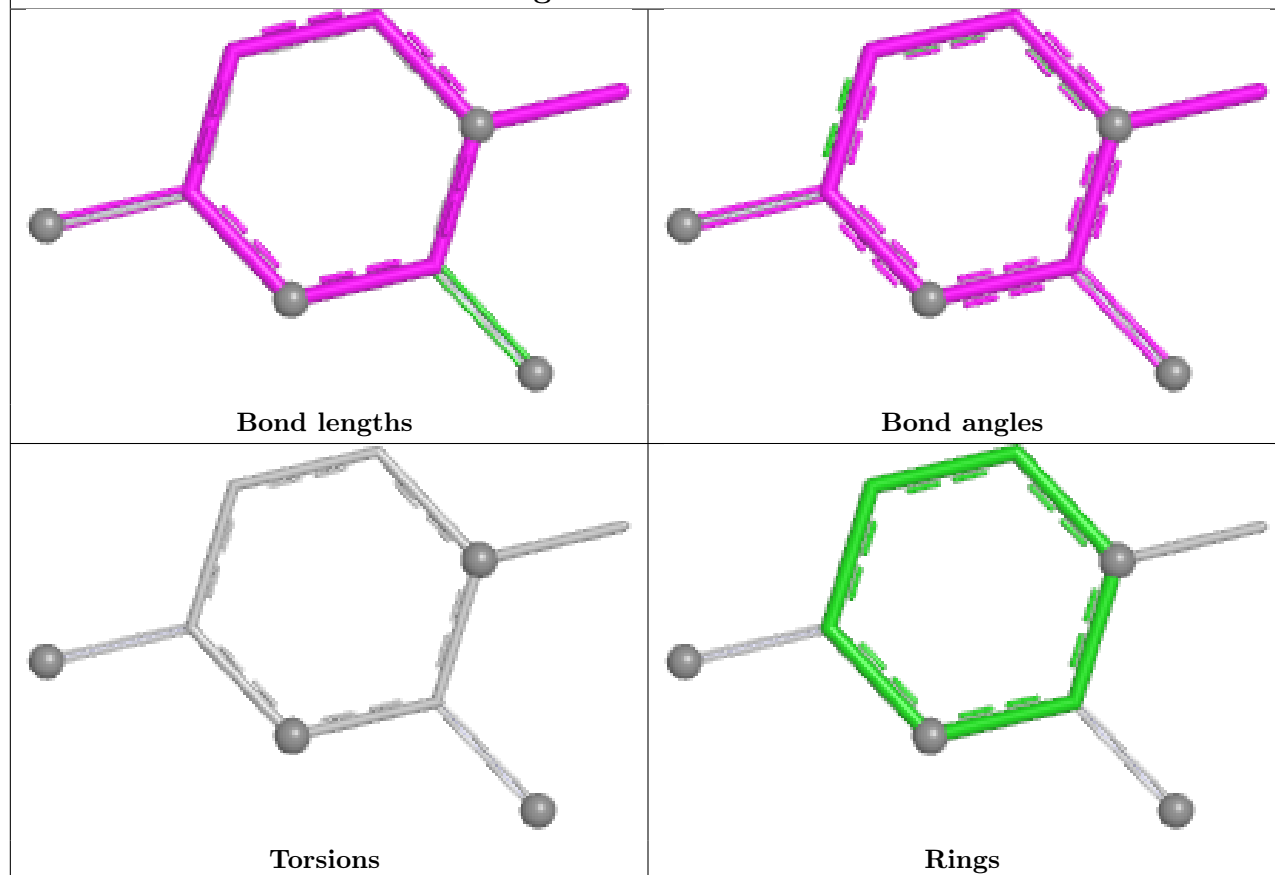
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	201	NAG	1	0
5	B	201	NAG	1	0
7	A	207[A]	CSQ	4	0
5	B	203	NAG	1	0
10	B	207	U5P	2	0
8	A	208[B]	CSV	7	0
9	A	209	1PE	11	0

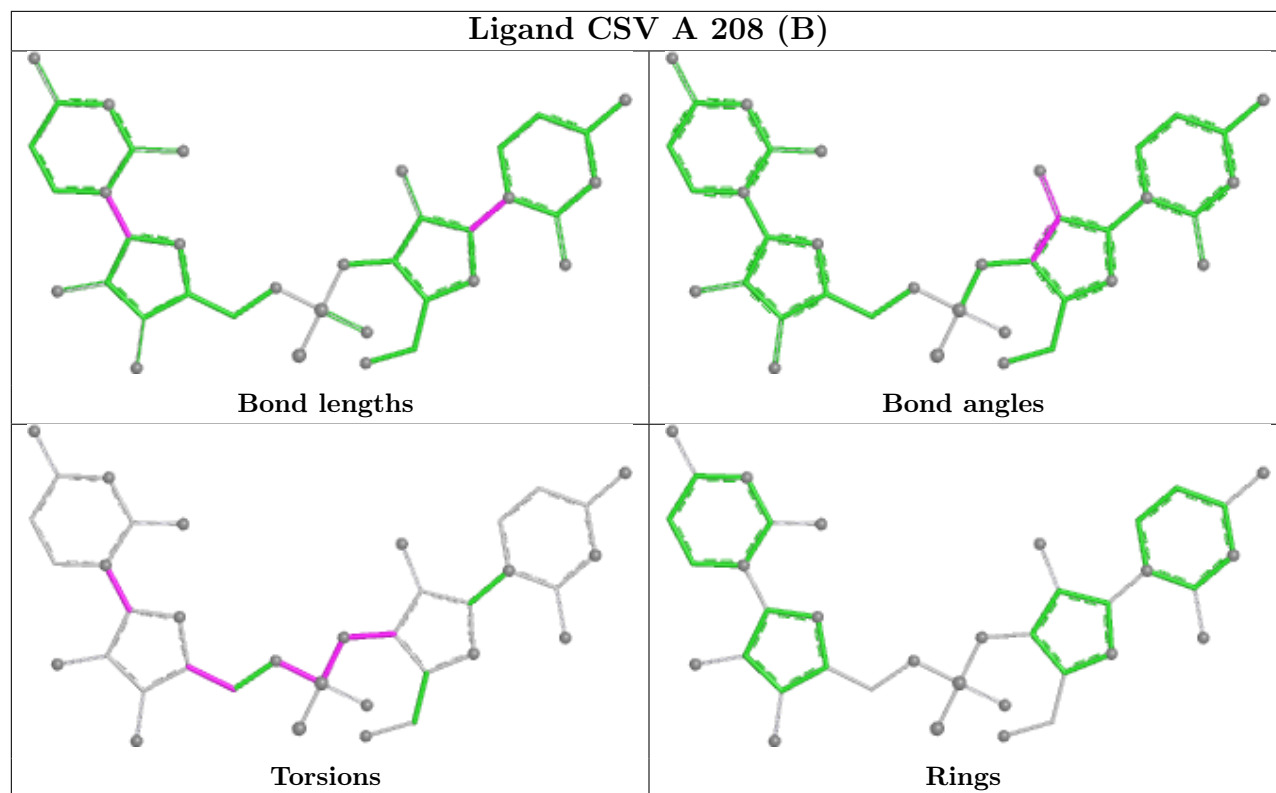
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand CSQ A 207 (A)



## Ligand U5P B 207





## 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	158/167 (94%)	0.13	9 (5%) 30 28	22, 38, 71, 93	9 (5%)
1	B	160/167 (95%)	0.52	16 (10%) 14 12	27, 46, 80, 98	10 (6%)
All	All	318/334 (95%)	0.33	25 (7%) 20 18	22, 41, 78, 98	19 (5%)

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	9.7
1	B	161	ILE	6.9
1	A	160[A]	GLU	6.0
1	A	109	LEU	5.3
1	B	107	GLN	4.6

### 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.

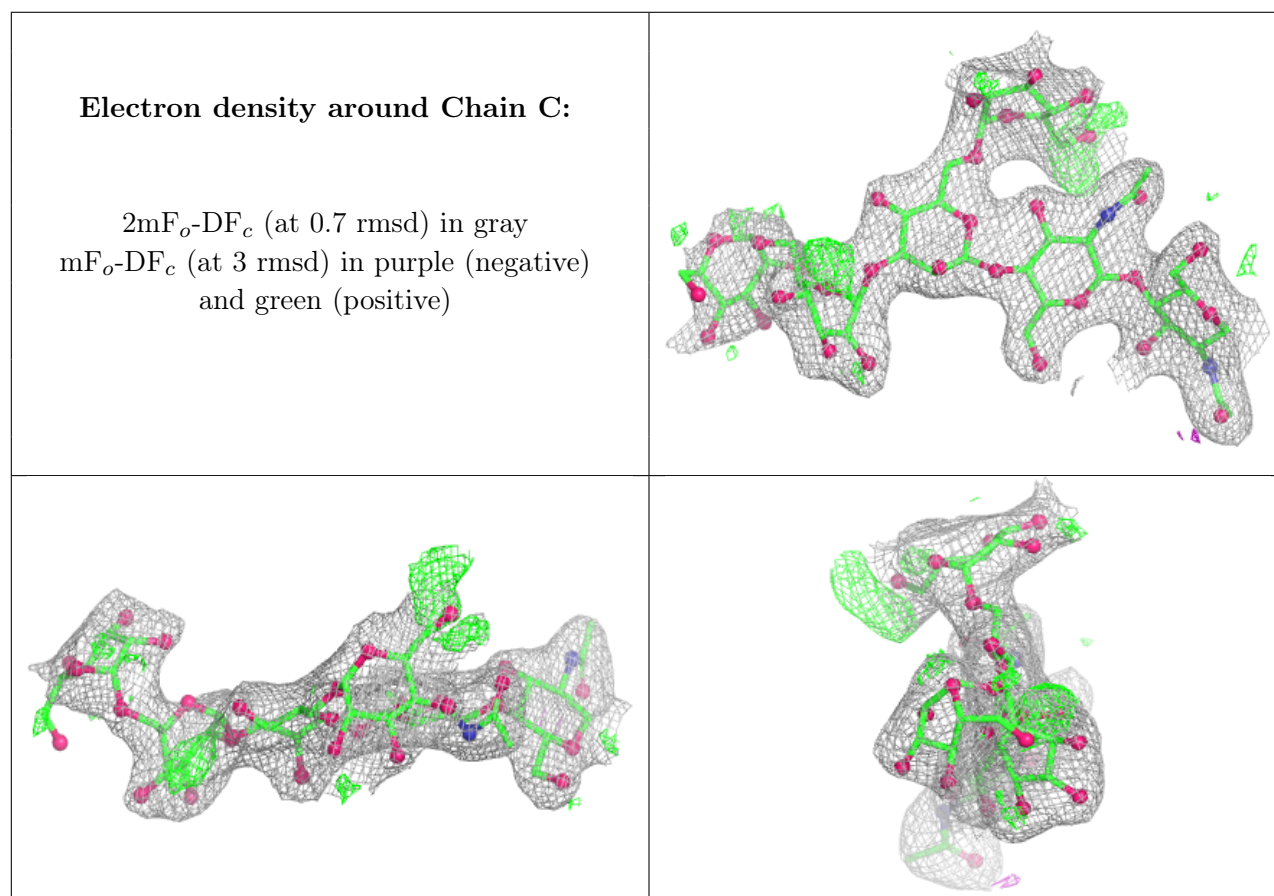
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	G	2	14/15	0.69	0.24	71,75,78,78	8
4	BMA	F	5	11/12	0.73	0.19	67,70,72,74	9
4	BMA	F	7	11/12	0.73	0.18	73,76,78,80	9
3	NAG	D	2	14/15	0.74	0.25	51,55,58,58	12
3	NAG	E	2	14/15	0.75	0.23	60,64,66,66	11

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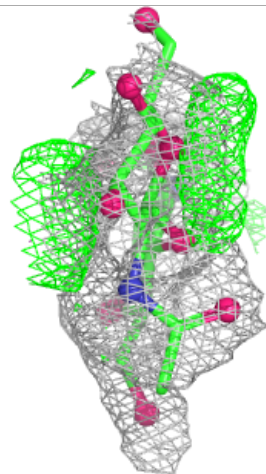
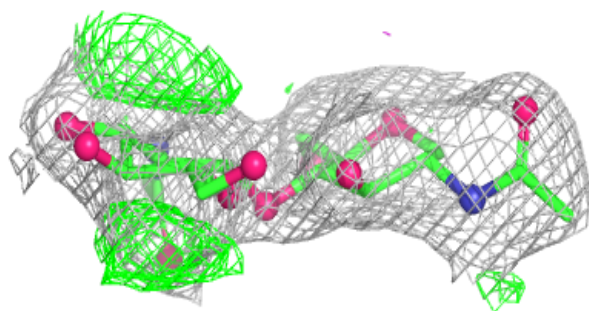
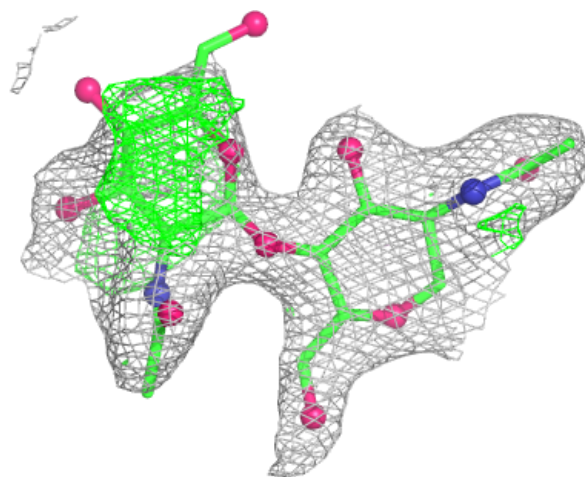
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BMA	C	5	11/12	0.76	0.25	71,75,77,78	8
2	BMA	C	6	11/12	0.83	0.15	62,65,67,68	5
4	MAN	F	6	11/12	0.84	0.19	63,67,70,73	6
3	NAG	G	1	14/15	0.84	0.20	61,65,67,68	5
3	NAG	E	1	14/15	0.87	0.16	50,54,57,57	8
2	BMA	C	4	11/12	0.91	0.18	55,59,61,67	6
4	BMA	F	4	11/12	0.92	0.13	54,57,59,64	4
4	BMA	F	3	11/12	0.92	0.11	46,49,52,58	6
4	NAG	F	1	14/15	0.94	0.09	34,38,40,41	7
3	NAG	D	1	14/15	0.94	0.12	41,45,48,49	6
2	BMA	C	3	11/12	0.95	0.10	45,49,52,57	2
2	NAG	C	1	14/15	0.96	0.08	33,37,39,40	6
2	NAG	C	2	14/15	0.96	0.09	35,39,41,42	5
4	NAG	F	2	14/15	0.97	0.08	36,40,42,43	3

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.



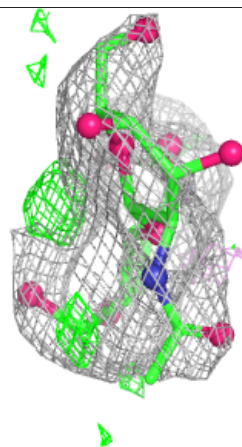
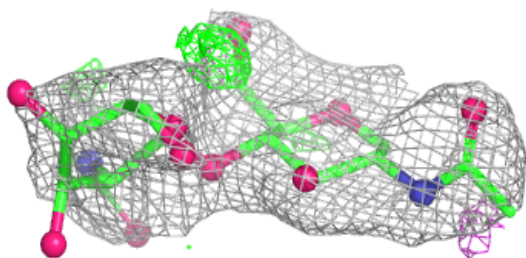
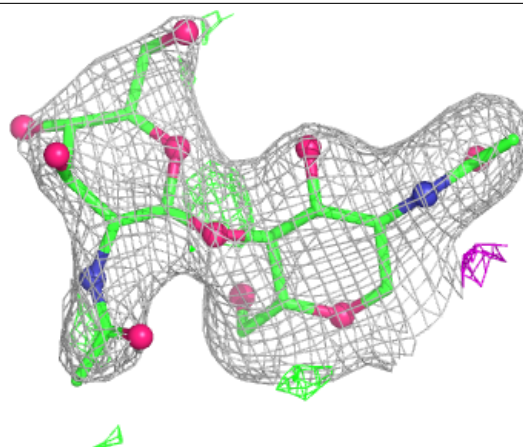
**Electron density around Chain D:**

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



**Electron density around Chain E:**

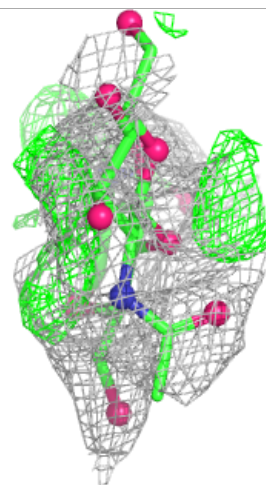
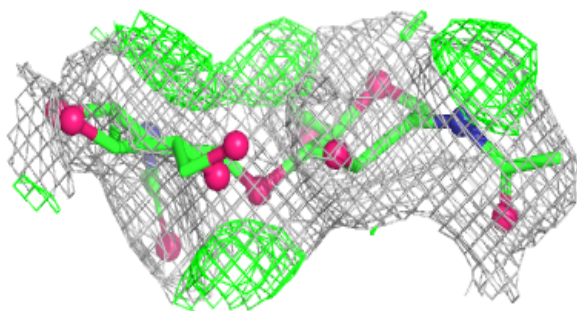
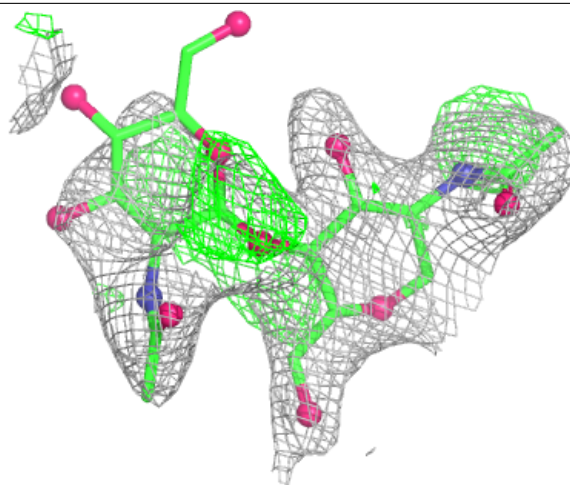
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



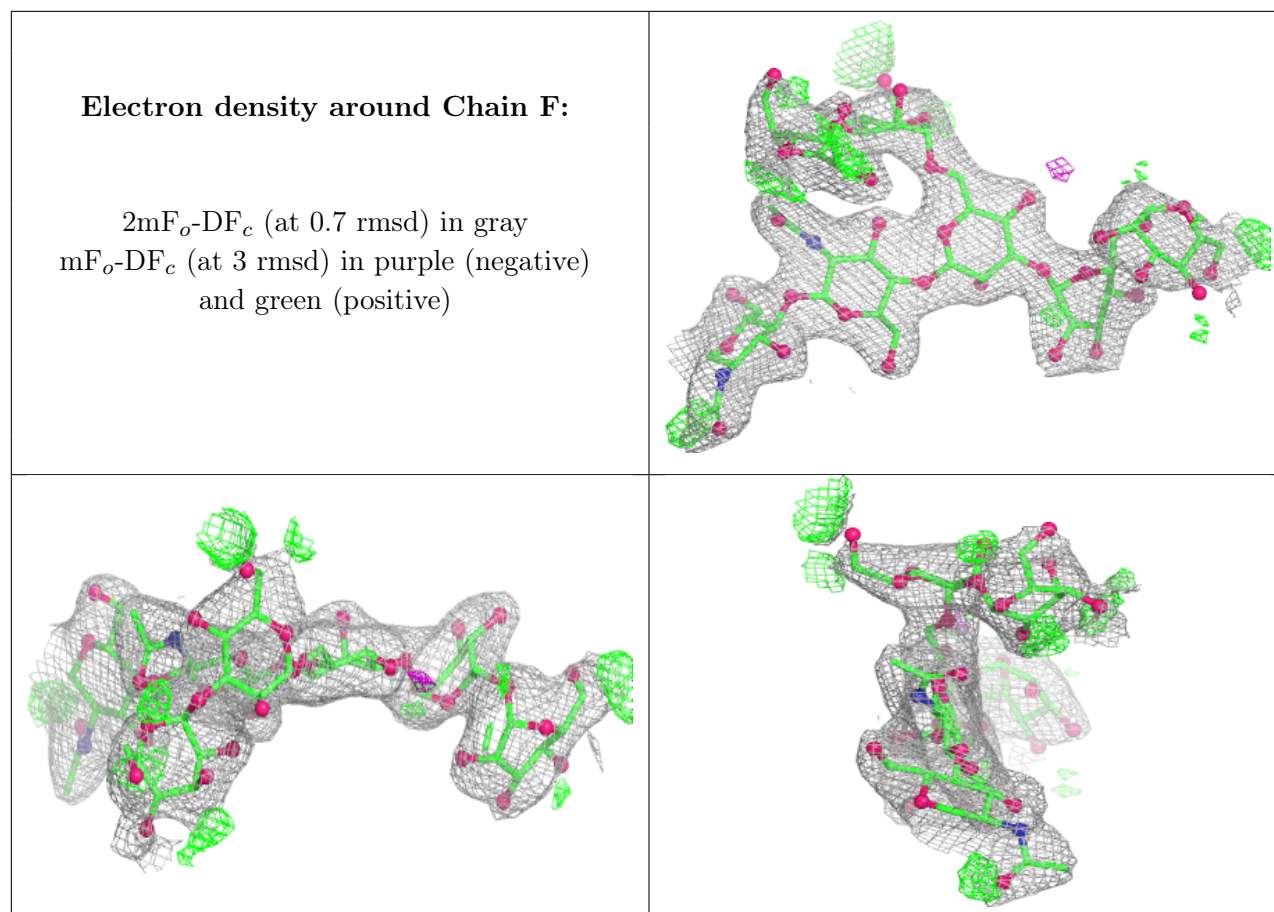


**Electron density around Chain G:**

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







## 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( $\text{\AA}^2$ )	Q<0.9
10	U5P	B	207	9/21	0.62	0.31	79,87,89,90	0
5	NAG	B	202	14/15	0.74	0.22	82,86,89,89	5
5	NAG	A	201	14/15	0.79	0.18	67,71,73,73	8
5	NAG	A	202	14/15	0.80	0.17	53,56,60,60	6
5	NAG	A	203	14/15	0.80	0.17	67,70,73,73	7
5	NAG	B	201	14/15	0.81	0.17	65,69,72,72	8
6	SO4	B	205	5/5	0.83	0.16	85,88,89,90	0
6	SO4	B	206	5/5	0.84	0.14	108,111,113,113	0
6	SO4	B	208	5/5	0.85	0.15	115,119,119,120	0
5	NAG	B	203	14/15	0.89	0.14	48,52,55,55	9
9	1PE	A	209	16/16	0.94	0.13	30,34,36,37	13
6	SO4	A	205	5/5	0.94	0.21	46,49,50,53	5

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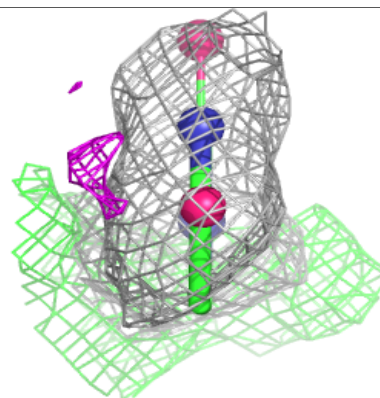
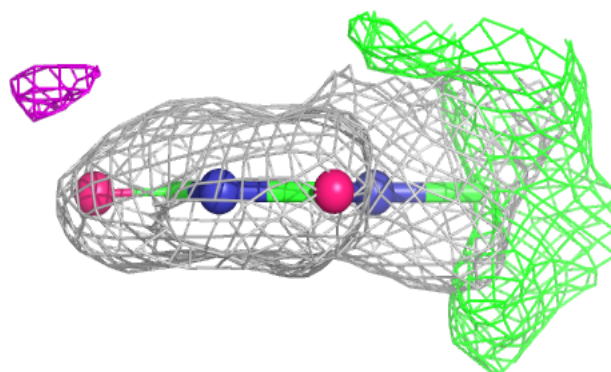
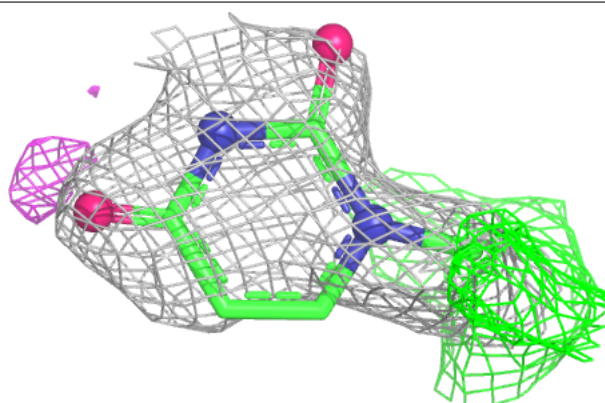
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	B	204	5/5	0.95	0.09	57,60,61,61	0
8	CSV	A	208[B]	37/37	0.97	0.06	22,29,37,43	37
6	SO4	A	206	5/5	0.97	0.07	48,49,54,56	0
7	CSQ	A	207[A]	37/37	0.97	0.09	30,49,54,55	37
6	SO4	A	204	5/5	0.99	0.05	36,36,39,41	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.

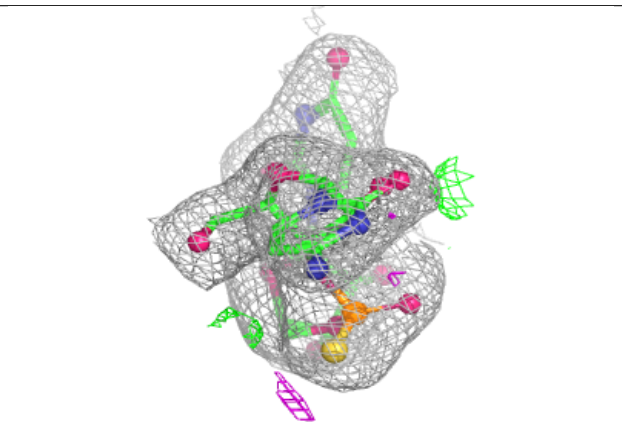
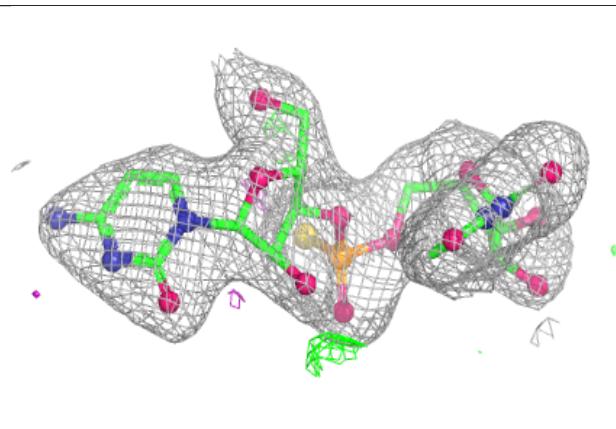
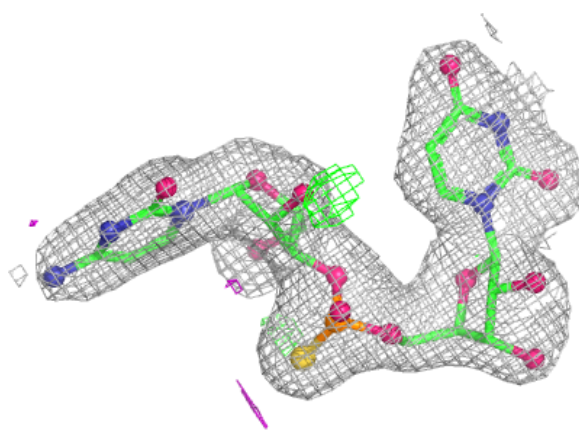
**Electron density around U5P B 207:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

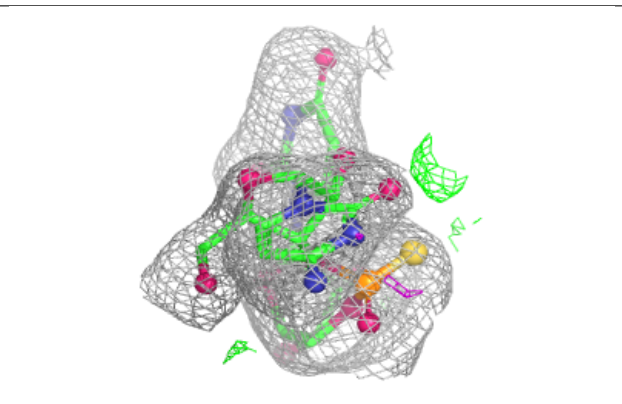
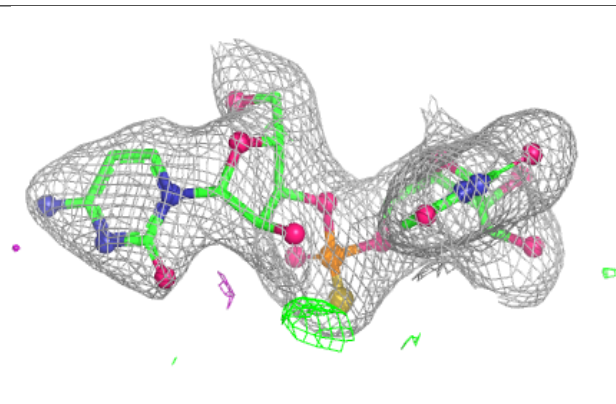
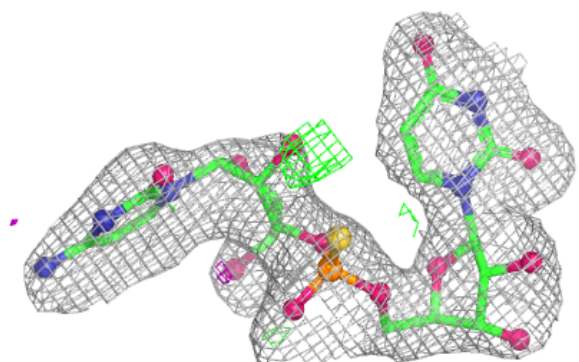


**Electron density around CSV A 208 (B):**

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

**Electron density around CSQ A 207 (A):**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.