



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 24, 2023 – 01:36 PM EDT

PDB ID : 5UGY  
Title : Influenza hemagglutinin in complex with a neutralizing antibody  
Authors : Whittle, J.R.R.; Jenni, S.; Harrison, S.C.  
Deposited on : 2017-01-10  
Resolution : 2.80 Å(reported)

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

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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

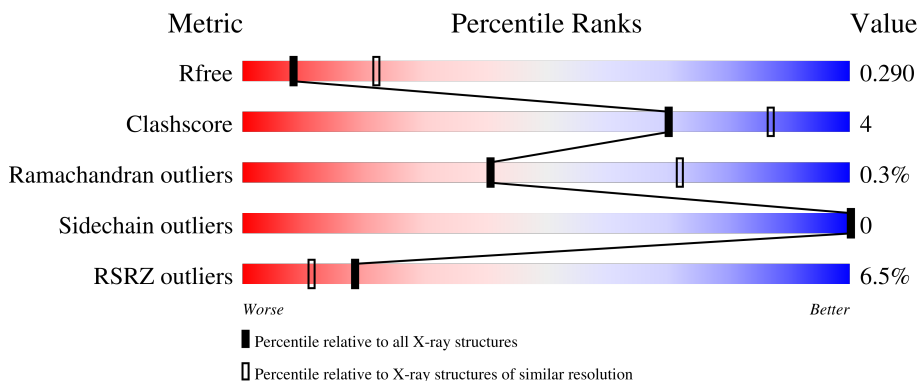
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	323	
1	C	323	
1	E	323	
2	B	173	
2	D	173	

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Mol	Chain	Length	Quality of chain
2	F	173	16% 88% 12%
3	H	227	2% 87% 11%
3	I	227	7% 88% 10%
3	J	227	4% 88% 9%
4	L	210	2% 90% 9%
4	M	210	2% 90% 9%
4	N	210	2% 89% 10%
5	G	2	100%
5	O	2	100%
5	P	2	100%
5	R	2	100%
5	S	2	100%
5	U	2	50% 50%
6	K	3	100%
6	Q	3	100%
6	T	3	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
5	NAG	G	2	-	-	-	X
5	NAG	O	2	-	-	-	X
5	NAG	P	2	-	-	-	X
5	NAG	R	1	-	-	-	X
5	NAG	R	2	-	-	-	X
5	NAG	S	2	-	-	-	X
5	NAG	U	1	-	-	-	X
5	NAG	U	2	-	-	-	X
7	NAG	A	406	-	-	-	X
7	NAG	A	407	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
7	NAG	C	407	-	-	-	X
7	NAG	E	406	-	-	-	X
7	NAG	E	407	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 42918 atoms, of which 21036 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	323	4975	1597	2440	441	486	11	0	0	0
1	C	323	4975	1597	2440	441	486	11	0	0	0
1	E	323	4975	1597	2440	441	486	11	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	-	expression tag	UNP A7UPX0
C	4	GLU	-	expression tag	UNP A7UPX0
E	4	GLU	-	expression tag	UNP A7UPX0

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	173	2718	874	1324	238	275	7	0	0	0
2	D	173	2718	874	1324	238	275	7	0	0	0
2	F	173	2718	874	1324	238	275	7	0	0	0

- Molecule 3 is a protein called CH65 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	H	221	3294	1062	1617	279	328	8	0	0	0
3	I	221	3294	1062	1617	279	328	8	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	J	221	Total	C	H	N	O	S	0	0	0
			3294	1062	1617	279	328	8			

- Molecule 4 is a protein called CH65 light chain.

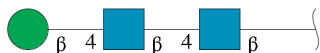
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
4	L	210	Total	C	H	N	O	S	0	0	0
			3078	973	1513	269	318	5			
4	M	210	Total	C	H	N	O	S	0	0	0
			3078	973	1513	269	318	5			
4	N	210	Total	C	H	N	O	S	0	0	0
			3078	973	1513	269	318	5			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



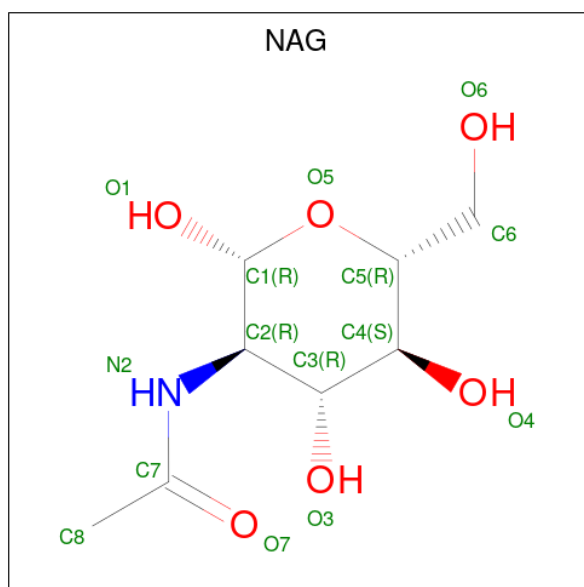
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	G	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
5	O	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
5	P	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
5	R	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
5	S	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
5	U	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 6 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
6	K	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			
6	Q	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			
6	T	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

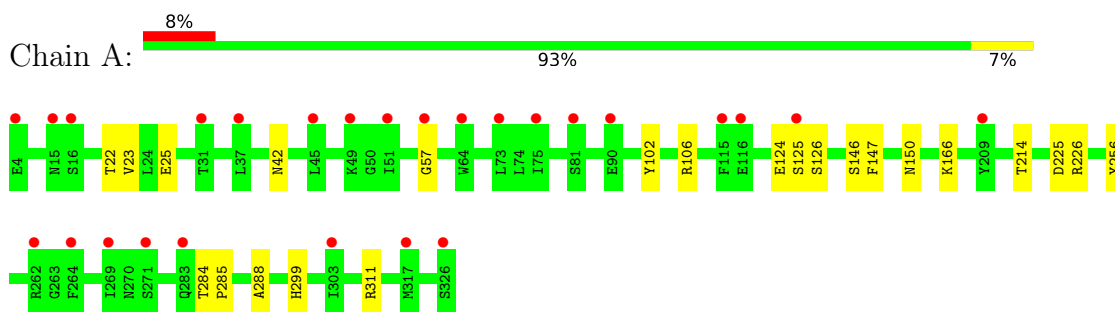


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
7	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
7	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
7	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
7	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
7	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

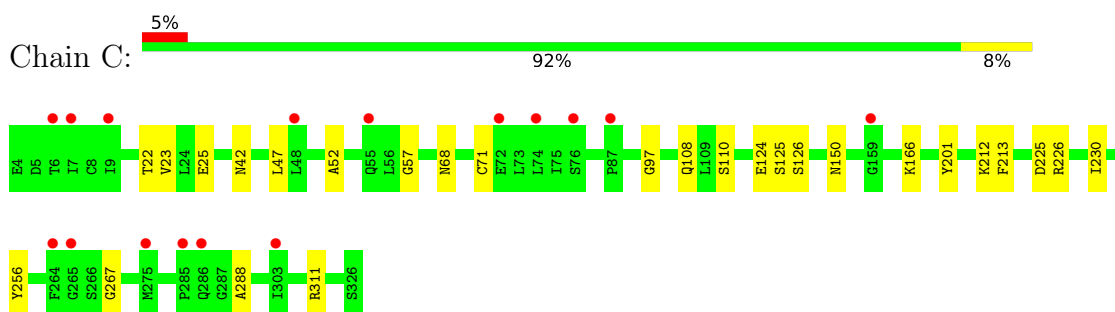
### 3 Residue-property plots [i](#)

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.

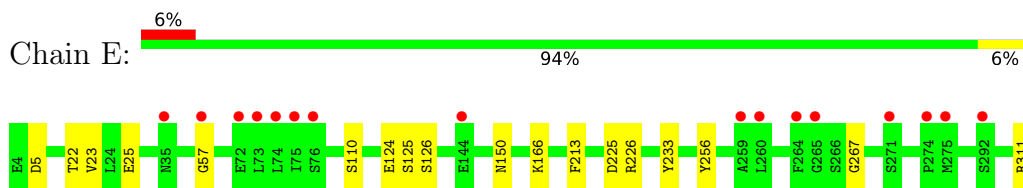
- Molecule 1: Hemagglutinin HA1



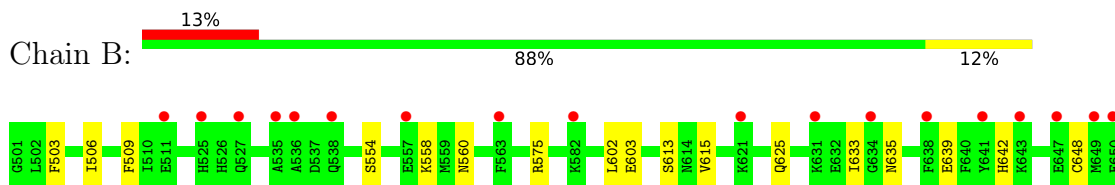
- Molecule 1: Hemagglutinin HA1



- Molecule 1: Hemagglutinin HA1



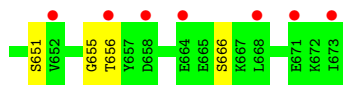
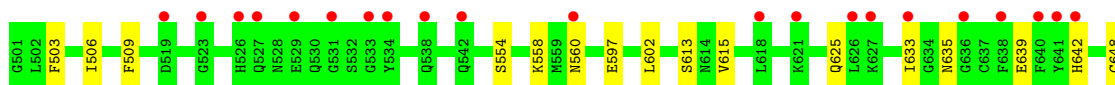
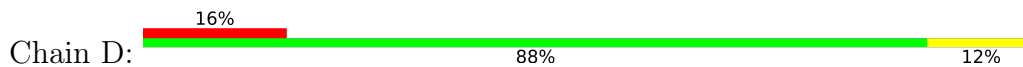
- Molecule 2: Hemagglutinin HA2



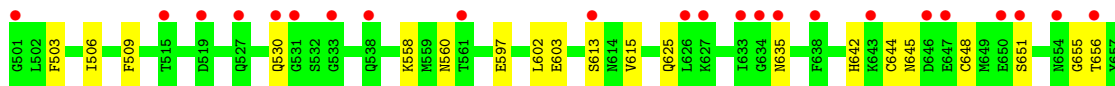
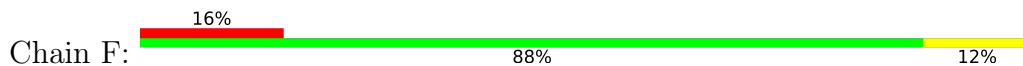




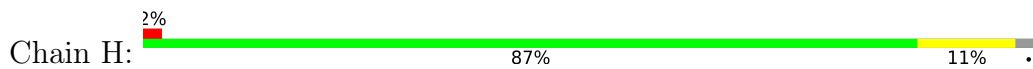
• Molecule 2: Hemagglutinin HA2



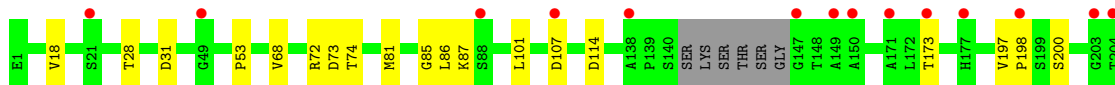
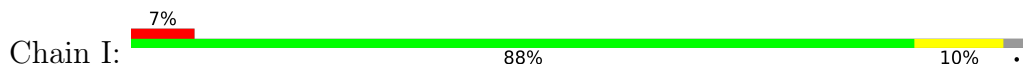
• Molecule 2: Hemagglutinin HA2



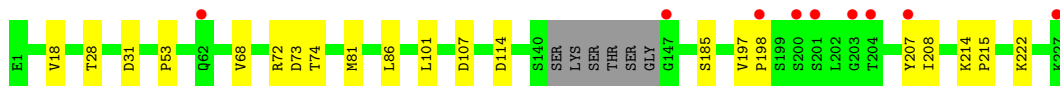
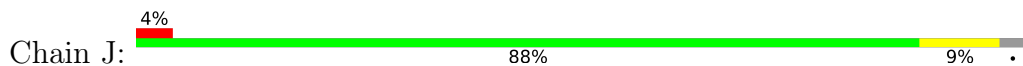
• Molecule 3: CH65 heavy chain



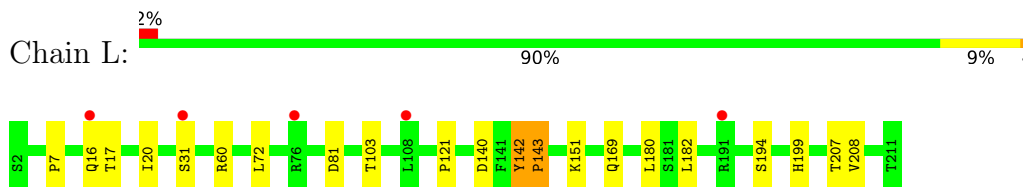
• Molecule 3: CH65 heavy chain



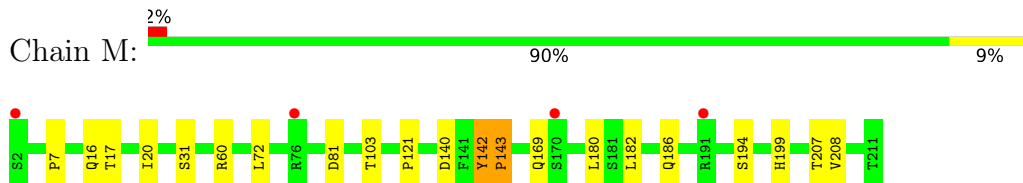
• Molecule 3: CH65 heavy chain



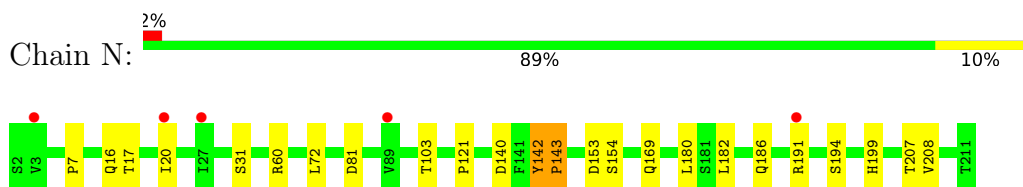
- Molecule 4: CH65 light chain



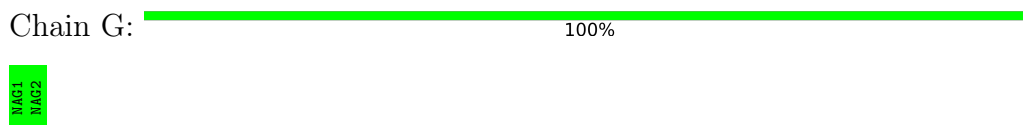
- Molecule 4: CH65 light chain



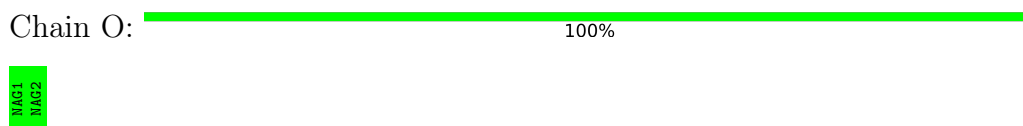
- Molecule 4: CH65 light chain



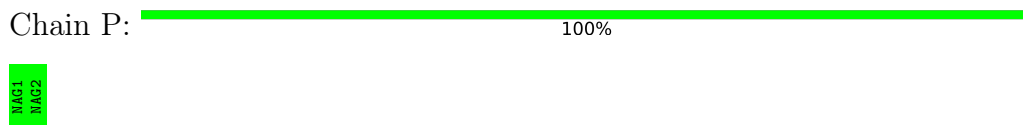
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  50% 50%MAG1  
MAG2

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

Chain K:  100%MAG1  
MAG2  
BMA3

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

Chain Q:  100%MAG1  
MAG2  
BMA3

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

Chain T:  100%MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.82Å 192.19Å 333.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.80 166.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.7 (29.92-2.80) 91.7 (166.61-2.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 2.82Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.259 , 0.289 0.261 , 0.290	Depositor DCC
$R_{free}$ test set	2754 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	42918	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: BMA, NAG

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	0.25	0/2601	0.47	0/3540
1	C	0.25	0/2601	0.47	0/3540
1	E	0.25	0/2601	0.47	0/3540
2	B	0.27	0/1421	0.46	0/1909
2	D	0.27	0/1421	0.46	0/1909
2	F	0.27	0/1421	0.46	0/1909
3	H	0.26	0/1722	0.49	0/2351
3	I	0.27	0/1722	0.50	0/2351
3	J	0.27	0/1722	0.49	0/2351
4	L	0.26	0/1603	0.50	0/2192
4	M	0.26	0/1603	0.50	0/2192
4	N	0.26	0/1603	0.50	0/2192
All	All	0.26	0/22041	0.48	0/29976

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
4	L	0	1
4	M	0	1
4	N	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	L	142	TYR	Peptide
4	M	142	TYR	Peptide
4	N	142	TYR	Peptide

## 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	2535	2440	2440	14	0
1	C	2535	2440	2440	16	0
1	E	2535	2440	2440	11	0
2	B	1394	1324	1323	16	0
2	D	1394	1324	1323	14	0
2	F	1394	1324	1323	17	0
3	H	1677	1617	1617	14	1
3	I	1677	1617	1617	13	2
3	J	1677	1617	1617	12	1
4	L	1565	1513	1513	14	0
4	M	1565	1513	1513	14	0
4	N	1565	1513	1513	17	0
5	G	28	27	25	0	0
5	O	28	27	25	0	0
5	P	28	27	25	0	0
5	R	28	27	25	0	0
5	S	28	27	25	0	0
5	U	28	27	25	0	0
6	K	39	36	34	0	0
6	Q	39	36	34	0	0
6	T	39	36	34	0	0
7	A	28	28	26	0	0
7	C	28	28	26	0	0
7	E	28	28	26	0	0
All	All	21882	21036	21009	155	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 155 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)
2:B:625:GLN:NE2	2:B:655:GLY:O	2.04	0.91
2:D:625:GLN:NE2	2:D:655:GLY:O	2.09	0.86
2:F:625:GLN:NE2	2:F:655:GLY:O	2.11	0.84
1:E:225:ASP:O	1:E:226:ARG:NH1	2.12	0.81
1:C:225:ASP:O	1:C:226:ARG:NH1	2.13	0.79

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:173:THR:OG1	3:I:173:THR:OG1[8_555]	2.11	0.09
3:I:200:SER:OG	3:J:185:SER:OG[3_545]	2.13	0.07

## 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	321/323 (99%)	304 (95%)	16 (5%)	1 (0%)	41	72
1	C	321/323 (99%)	305 (95%)	15 (5%)	1 (0%)	41	72
1	E	321/323 (99%)	305 (95%)	15 (5%)	1 (0%)	41	72
2	B	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
2	D	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
2	F	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
3	H	217/227 (96%)	205 (94%)	12 (6%)	0	100	100
3	I	217/227 (96%)	207 (95%)	10 (5%)	0	100	100
3	J	217/227 (96%)	206 (95%)	11 (5%)	0	100	100
4	L	208/210 (99%)	196 (94%)	10 (5%)	2 (1%)	15	44
4	M	208/210 (99%)	197 (95%)	9 (4%)	2 (1%)	15	44
4	N	208/210 (99%)	197 (95%)	9 (4%)	2 (1%)	15	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2751/2799 (98%)	2593 (94%)	149 (5%)	9 (0%)	41	72

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	143	PRO
4	M	143	PRO
4	N	143	PRO
4	L	31	SER
4	M	31	SER

### 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	283/283 (100%)	283 (100%)	0	100	100
1	C	283/283 (100%)	283 (100%)	0	100	100
1	E	283/283 (100%)	283 (100%)	0	100	100
2	B	149/149 (100%)	149 (100%)	0	100	100
2	D	149/149 (100%)	149 (100%)	0	100	100
2	F	149/149 (100%)	149 (100%)	0	100	100
3	H	185/190 (97%)	185 (100%)	0	100	100
3	I	185/190 (97%)	185 (100%)	0	100	100
3	J	185/190 (97%)	185 (100%)	0	100	100
4	L	177/177 (100%)	177 (100%)	0	100	100
4	M	177/177 (100%)	177 (100%)	0	100	100
4	N	177/177 (100%)	177 (100%)	0	100	100
All	All	2382/2397 (99%)	2382 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are



no such sidechains identified.

### 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](#)

21 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	$\# Z  > 2$
5	NAG	G	1	1,5	14,14,15	0.28	0	17,19,21	0.46	0
5	NAG	G	2	5	14,14,15	0.25	0	17,19,21	0.42	0
6	NAG	K	1	1,6	14,14,15	0.18	0	17,19,21	0.41	0
6	NAG	K	2	6	14,14,15	0.21	0	17,19,21	0.38	0
6	BMA	K	3	6	11,11,12	0.56	0	15,15,17	1.05	0
5	NAG	O	1	1,5	14,14,15	0.31	0	17,19,21	0.61	0
5	NAG	O	2	5	14,14,15	0.19	0	17,19,21	0.48	0
5	NAG	P	1	1,5	14,14,15	0.25	0	17,19,21	0.48	0
5	NAG	P	2	5	14,14,15	0.24	0	17,19,21	0.41	0
6	NAG	Q	1	1,6	14,14,15	0.18	0	17,19,21	0.42	0
6	NAG	Q	2	6	14,14,15	0.23	0	17,19,21	0.40	0
6	BMA	Q	3	6	11,11,12	0.57	0	15,15,17	1.04	0
5	NAG	R	1	1,5	14,14,15	0.28	0	17,19,21	0.65	0
5	NAG	R	2	5	14,14,15	0.17	0	17,19,21	0.47	0
5	NAG	S	1	1,5	14,14,15	0.26	0	17,19,21	0.46	0
5	NAG	S	2	5	14,14,15	0.26	0	17,19,21	0.41	0
6	NAG	T	1	1,6	14,14,15	0.18	0	17,19,21	0.42	0
6	NAG	T	2	6	14,14,15	0.21	0	17,19,21	0.40	0
6	BMA	T	3	6	11,11,12	0.59	0	15,15,17	1.04	0
5	NAG	U	1	1,5	14,14,15	0.31	0	17,19,21	0.63	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	U	2	5	14,14,15	0.19	0	17,19,21	0.47	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
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	1/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
5	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	1/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	0/2/19/22	0/1/1/1
5	NAG	R	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	NAG	S	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	1/6/23/26	0/1/1/1
6	BMA	T	3	6	-	0/2/19/22	0/1/1/1
5	NAG	U	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	1	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

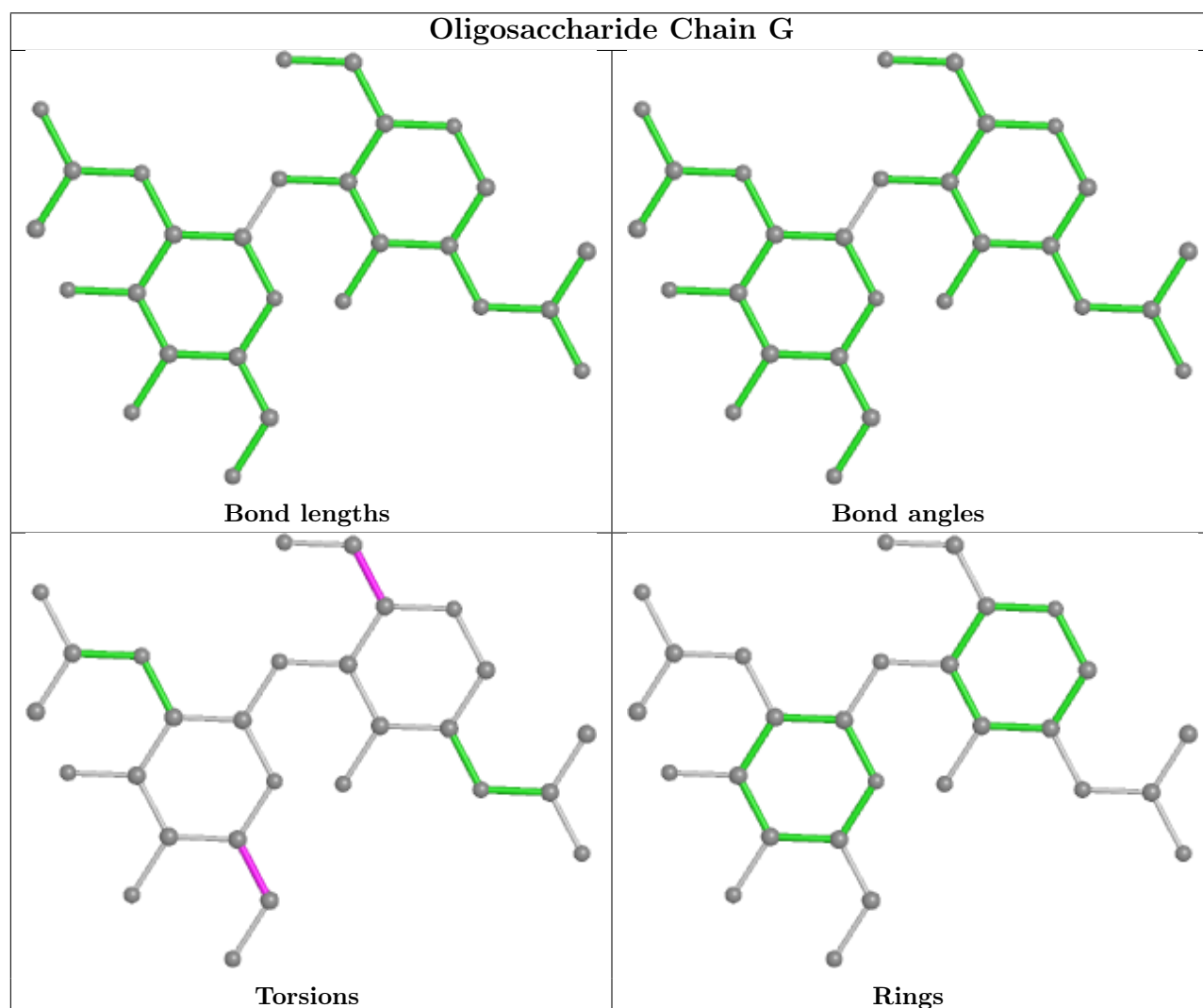
5 of 27 torsion outliers are listed below:

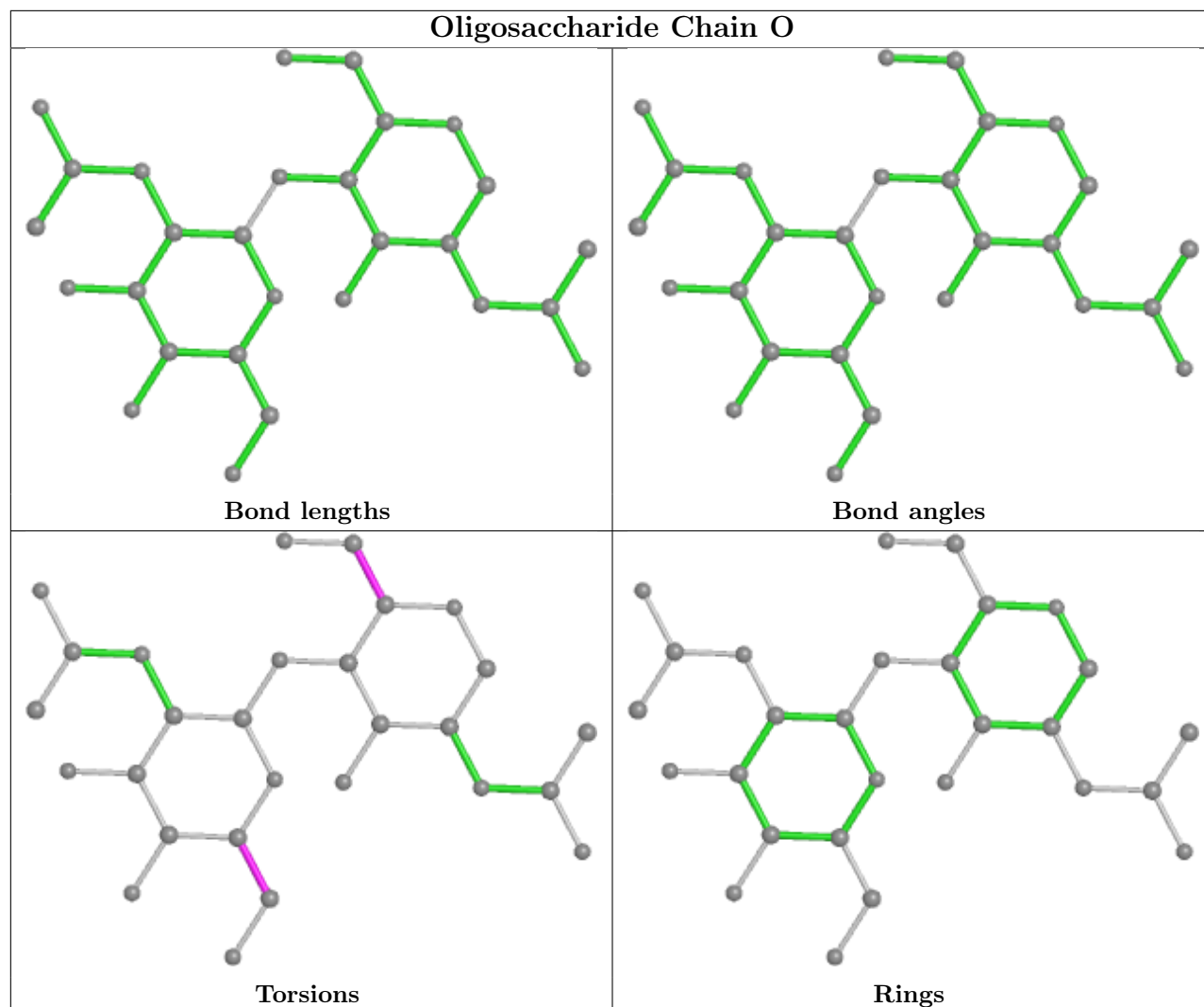
Mol	Chain	Res	Type	Atoms
5	G	1	NAG	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6

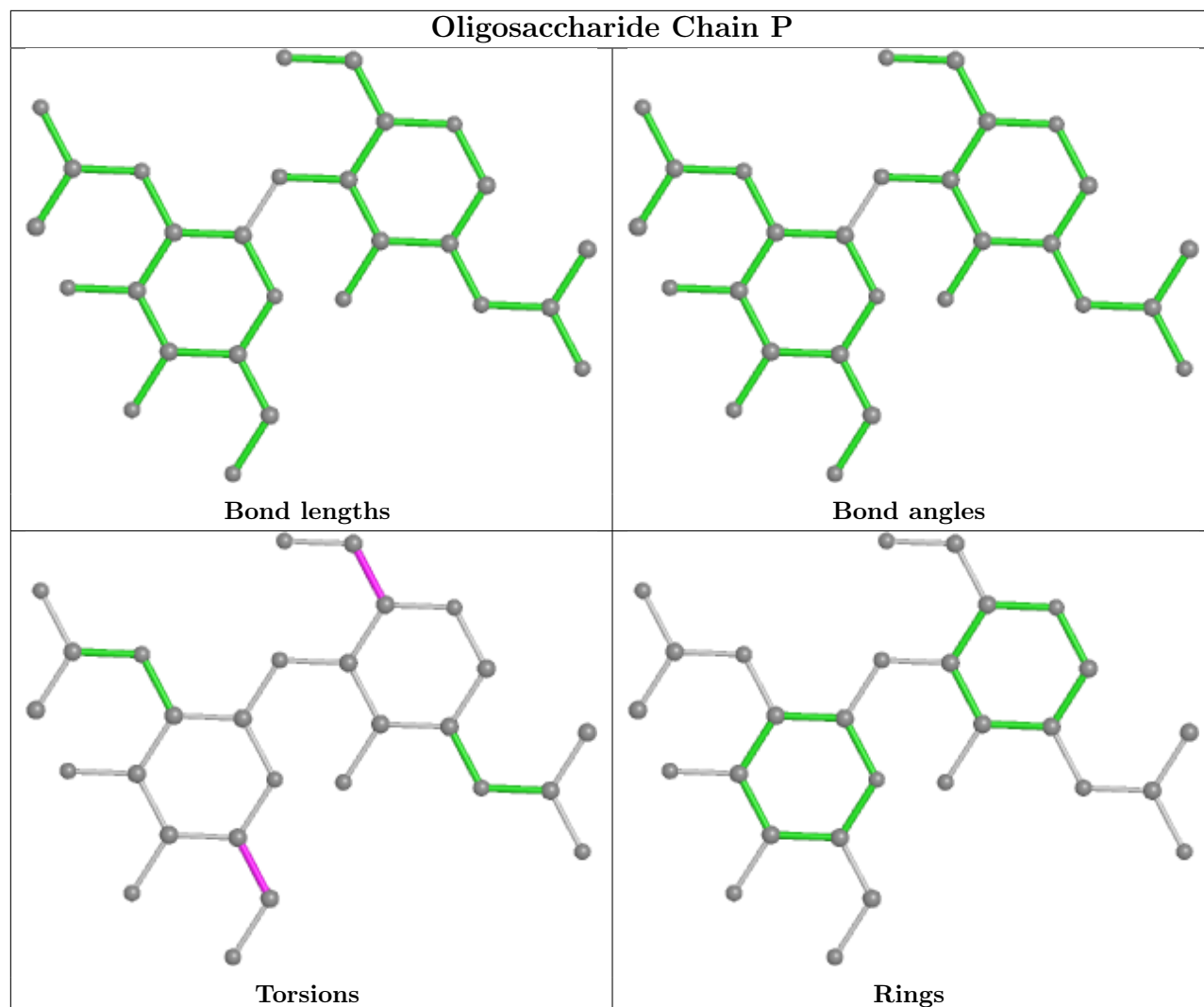
There are no ring outliers.

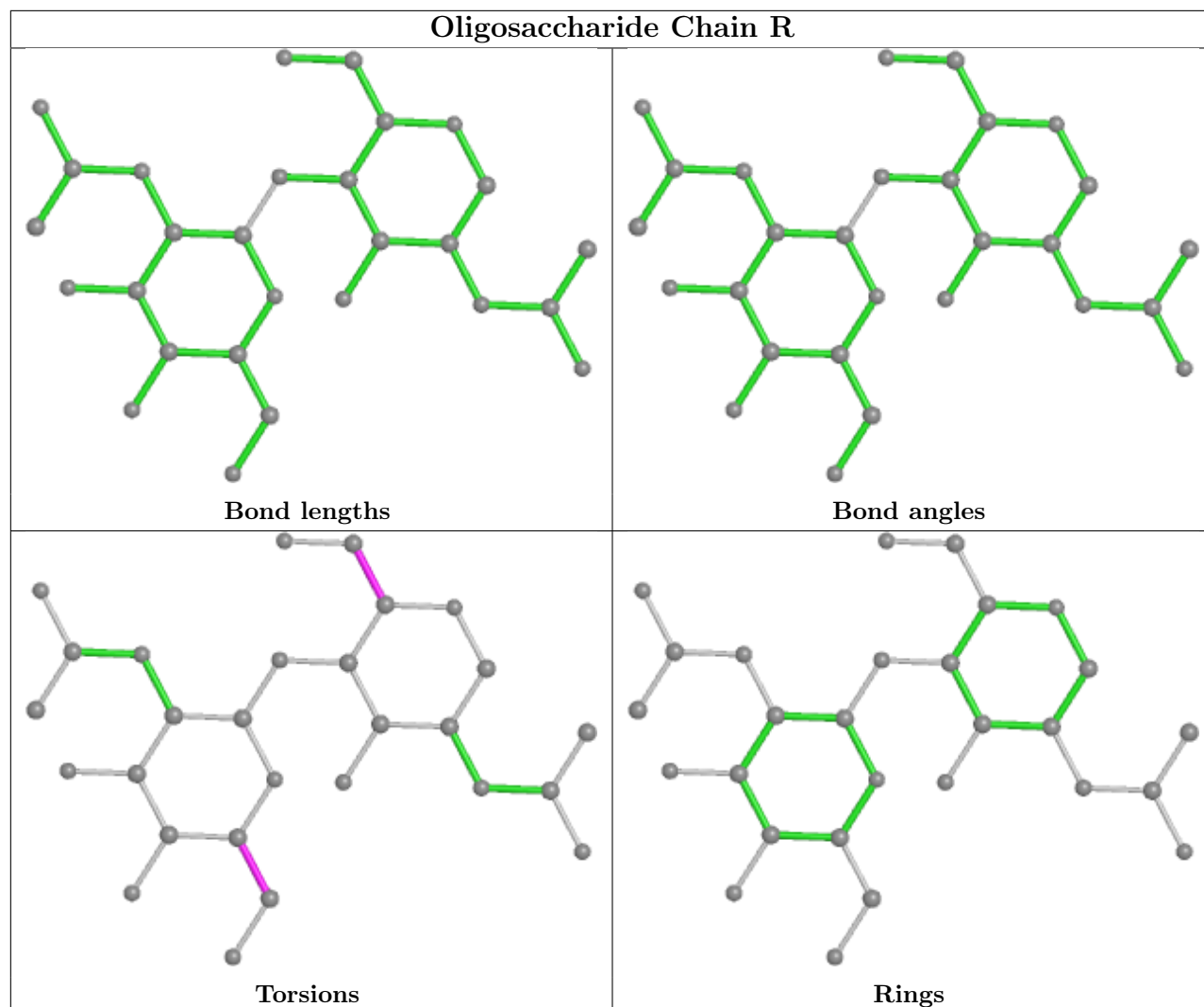
No monomer is involved in short contacts.

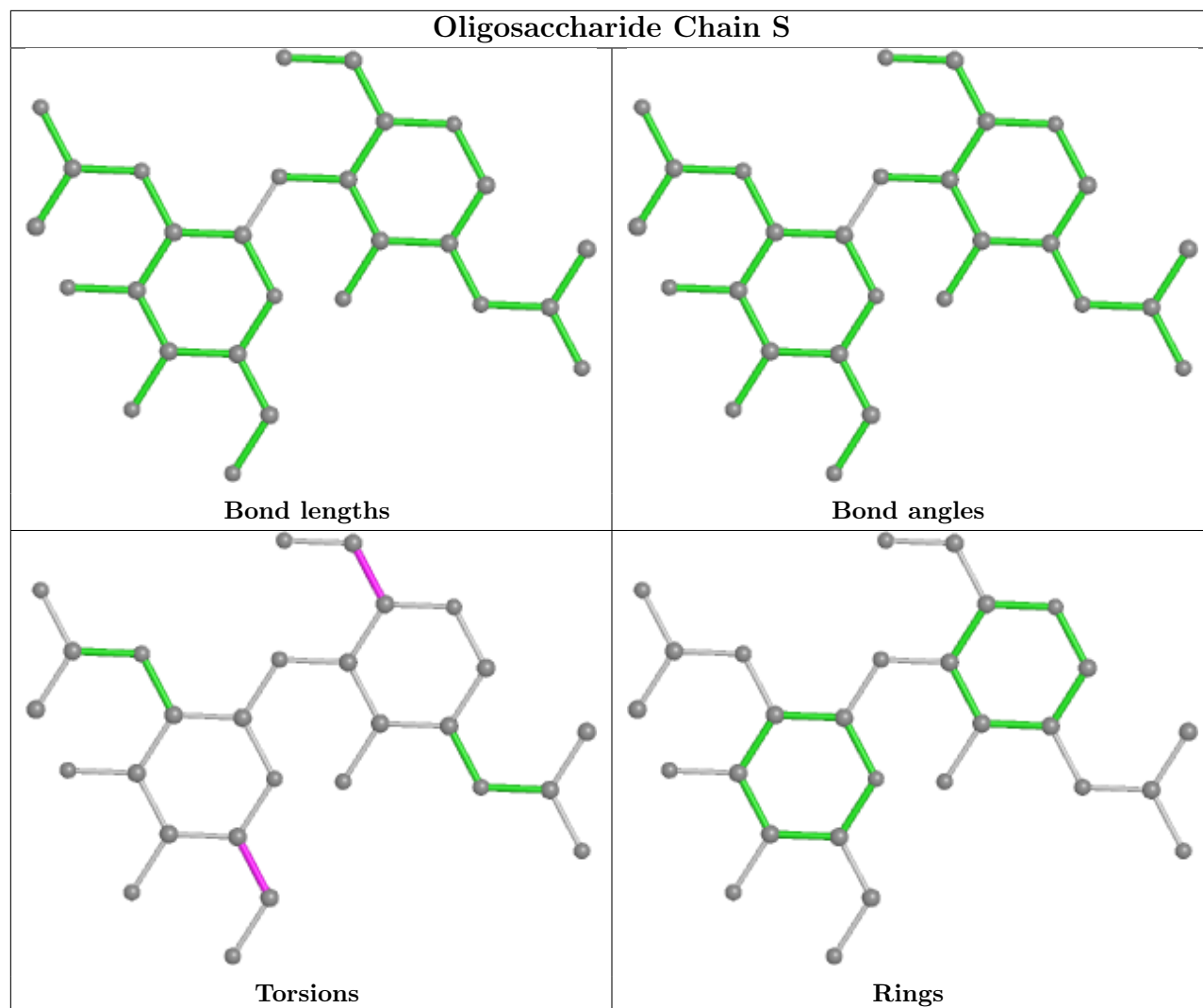
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

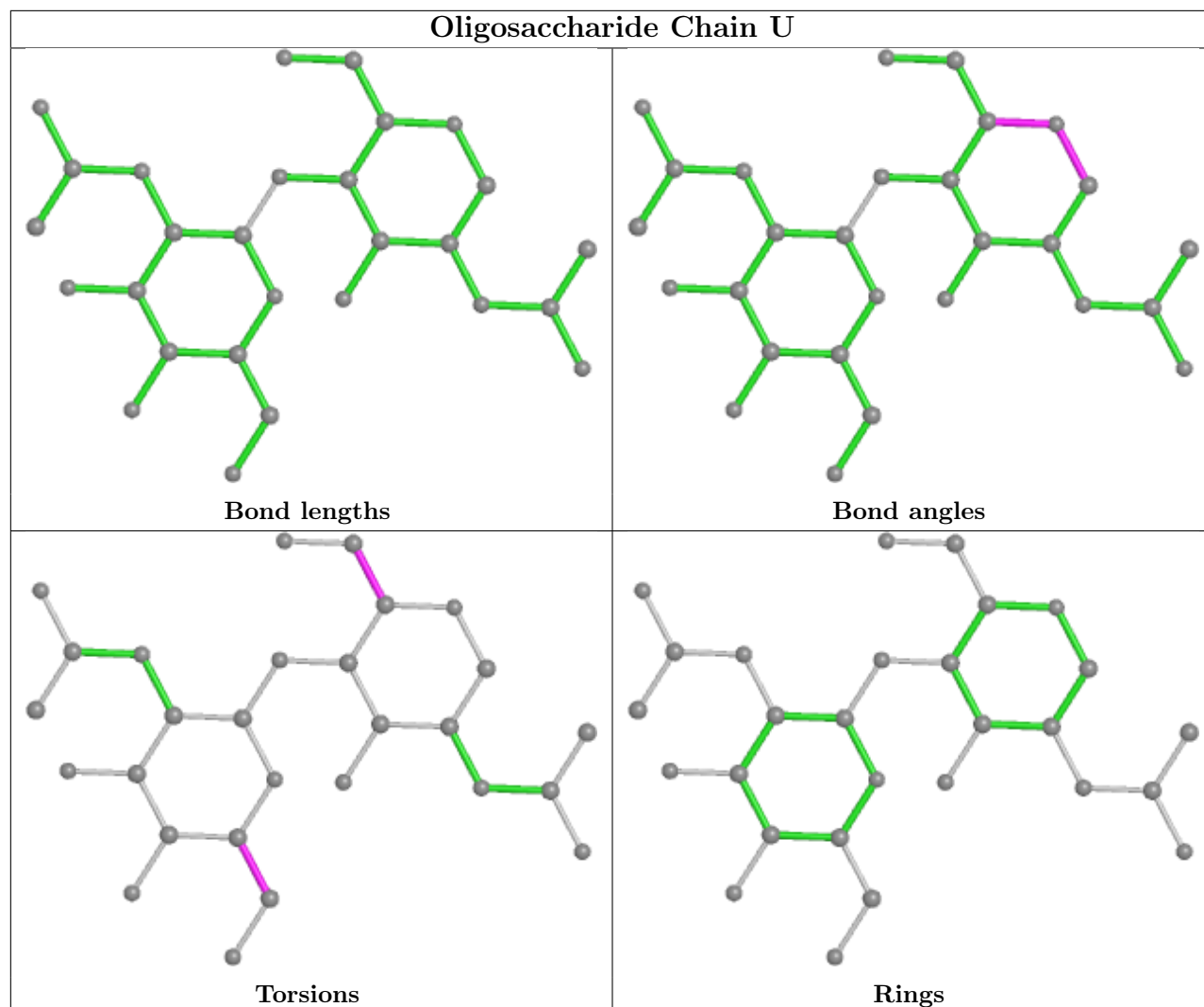




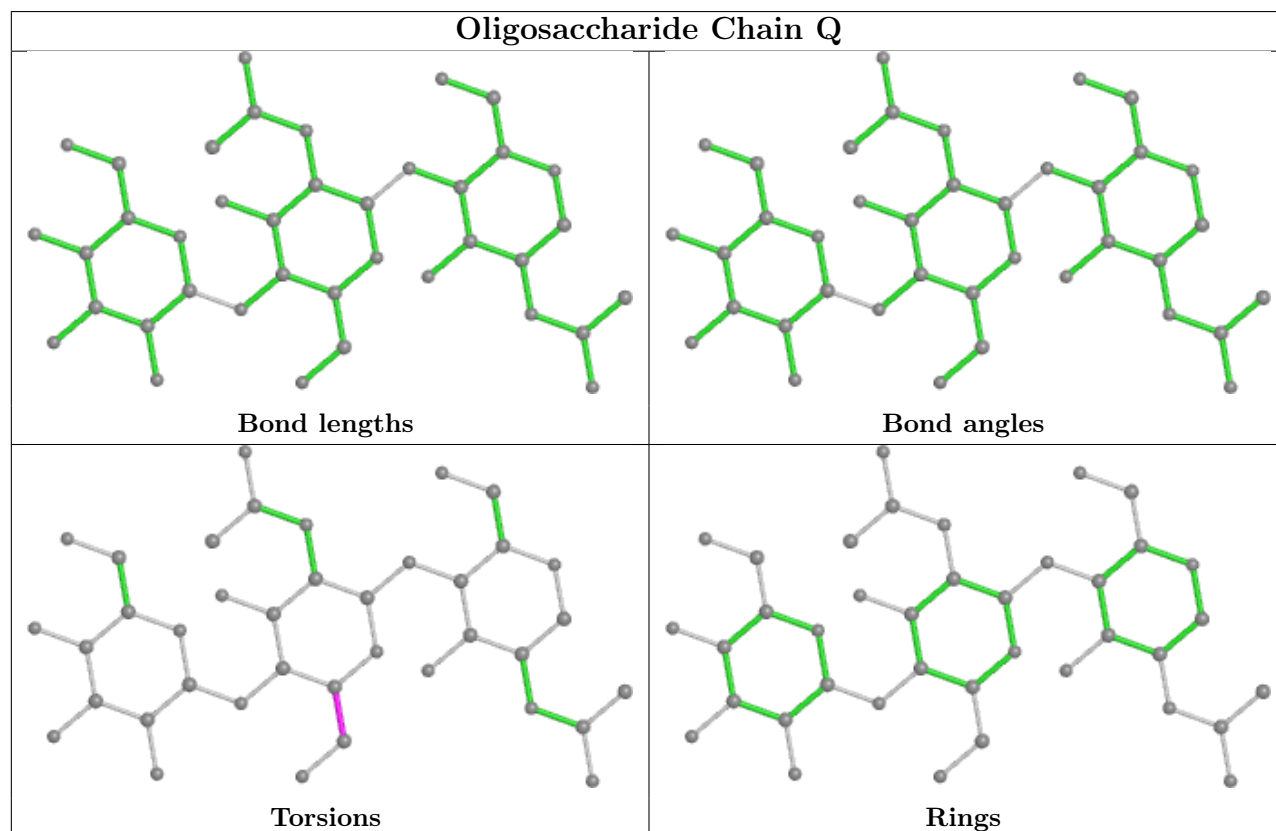
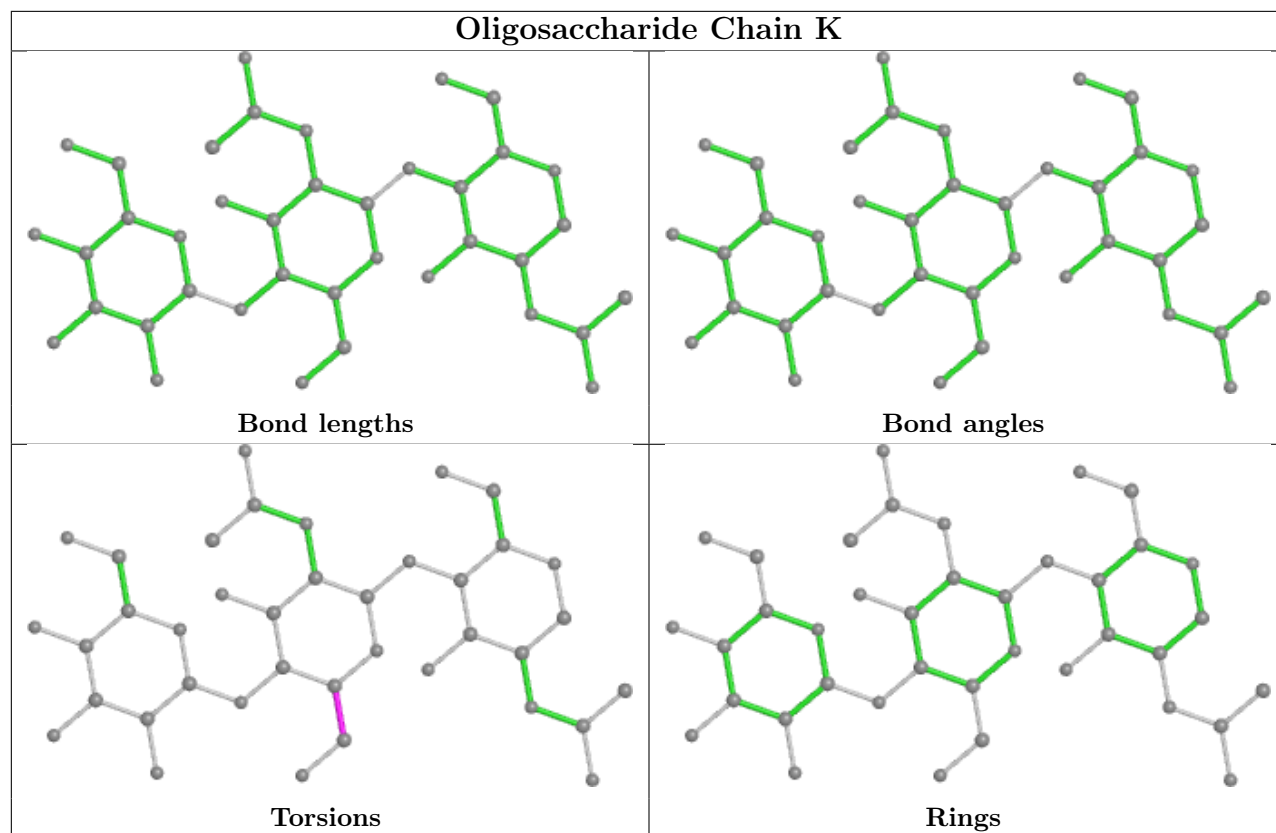


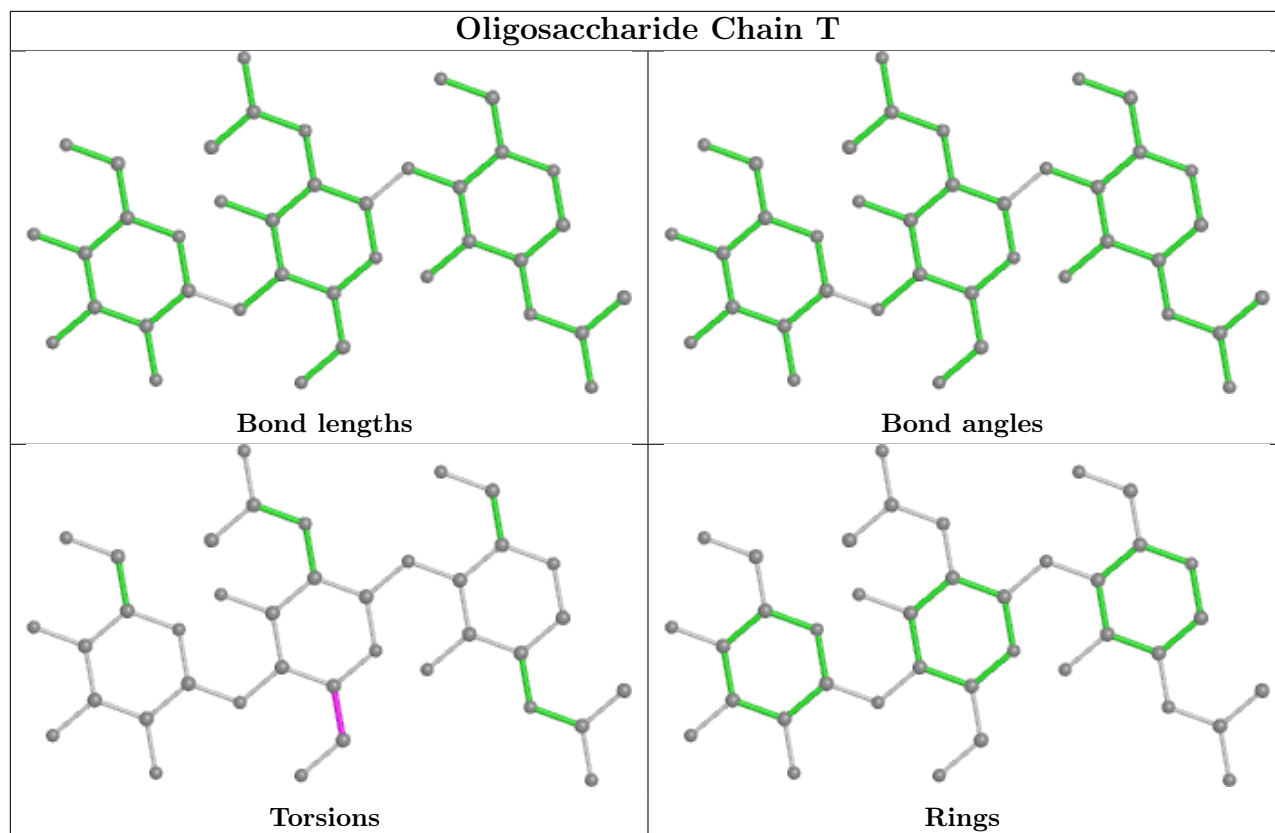












## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
7	NAG	A	406	1	14,14,15	0.25	0	17,19,21	0.50	0
7	NAG	E	407	1	14,14,15	0.16	0	17,19,21	0.44	0
7	NAG	A	407	1	14,14,15	0.15	0	17,19,21	0.45	0
7	NAG	E	406	1	14,14,15	0.24	0	17,19,21	0.50	0
7	NAG	C	406	1	14,14,15	0.25	0	17,19,21	0.48	0
7	NAG	C	407	1	14,14,15	0.17	0	17,19,21	0.45	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
7	NAG	A	406	1	-	2/6/23/26	0/1/1/1
7	NAG	E	407	1	-	0/6/23/26	0/1/1/1
7	NAG	A	407	1	-	0/6/23/26	0/1/1/1
7	NAG	E	406	1	-	2/6/23/26	0/1/1/1
7	NAG	C	406	1	-	1/6/23/26	0/1/1/1
7	NAG	C	407	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	406	NAG	O5-C5-C6-O6
7	E	406	NAG	O5-C5-C6-O6
7	C	406	NAG	O5-C5-C6-O6
7	A	406	NAG	C4-C5-C6-O6
7	E	406	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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	323/323 (100%)	0.79	26 (8%) 12 6	31, 51, 78, 104	0
1	C	323/323 (100%)	0.67	16 (4%) 28 19	17, 38, 70, 99	0
1	E	323/323 (100%)	0.69	18 (5%) 24 16	17, 36, 70, 106	0
2	B	173/173 (100%)	1.02	23 (13%) 3 2	18, 54, 91, 108	0
2	D	173/173 (100%)	1.15	28 (16%) 1 1	12, 54, 103, 123	0
2	F	173/173 (100%)	1.09	28 (16%) 1 1	16, 45, 108, 114	0
3	H	221/227 (97%)	0.56	4 (1%) 68 61	15, 33, 57, 81	0
3	I	221/227 (97%)	0.70	15 (6%) 17 10	13, 28, 75, 106	0
3	J	221/227 (97%)	0.62	9 (4%) 37 27	12, 28, 67, 90	0
4	L	210/210 (100%)	0.65	5 (2%) 59 49	26, 51, 77, 103	0
4	M	210/210 (100%)	0.60	4 (1%) 66 59	20, 42, 67, 96	0
4	N	210/210 (100%)	0.61	5 (2%) 59 49	16, 36, 58, 78	0
All	All	2781/2799 (99%)	0.74	181 (6%) 18 11	12, 40, 83, 123	0

The worst 5 of 181 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	673	ILE	8.9
2	D	527	GLN	7.7
1	A	326	SER	7.1
1	E	75	ILE	5.6
2	D	533	GLY	5.5

### 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](#)

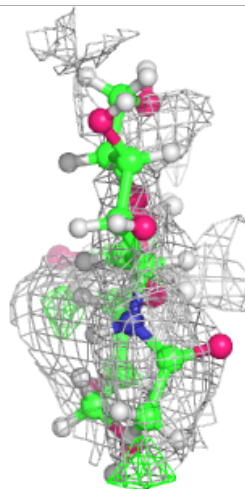
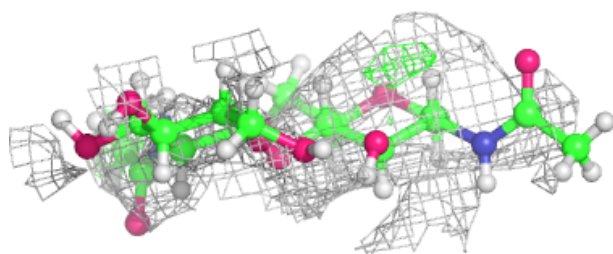
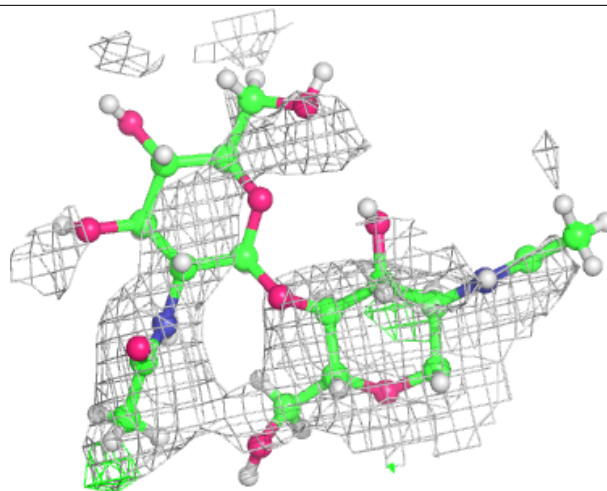
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

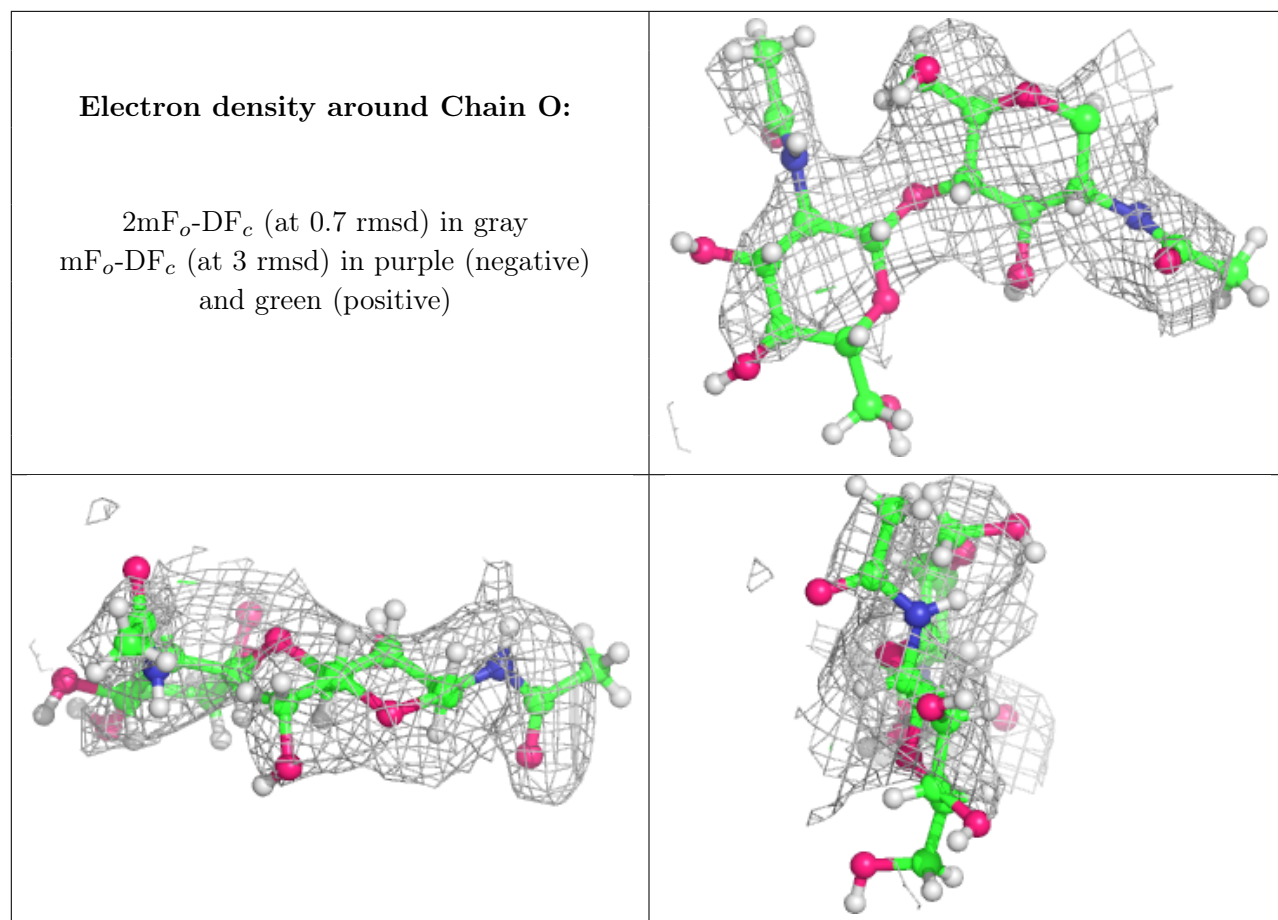
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	P	2	14/15	0.42	0.56	85,134,170,175	0
5	NAG	G	2	14/15	0.47	0.42	67,127,159,164	0
5	NAG	S	2	14/15	0.48	0.49	81,127,159,167	0
5	NAG	R	2	14/15	0.50	0.69	82,115,142,153	0
5	NAG	P	1	14/15	0.61	0.40	91,111,135,155	0
5	NAG	U	2	14/15	0.66	0.75	61,123,160,162	0
5	NAG	R	1	14/15	0.67	0.46	61,87,116,133	0
5	NAG	O	2	14/15	0.68	0.56	55,110,137,139	0
5	NAG	G	1	14/15	0.69	0.34	76,116,140,147	0
5	NAG	U	1	14/15	0.75	0.47	50,81,120,127	0
6	BMA	K	3	11/12	0.75	0.39	74,97,115,138	0
6	BMA	Q	3	11/12	0.77	0.39	85,106,127,130	0
6	NAG	Q	2	14/15	0.78	0.37	50,97,117,124	0
6	NAG	K	2	14/15	0.78	0.32	55,92,118,125	0
6	BMA	T	3	11/12	0.79	0.24	64,98,117,123	0
5	NAG	O	1	14/15	0.83	0.29	56,87,110,121	0
5	NAG	S	1	14/15	0.83	0.25	73,97,122,140	0
6	NAG	T	2	14/15	0.86	0.29	51,82,101,117	0
6	NAG	K	1	14/15	0.90	0.28	40,73,120,125	0
6	NAG	Q	1	14/15	0.91	0.24	33,60,97,103	0
6	NAG	T	1	14/15	0.92	0.28	36,56,93,103	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 G:**

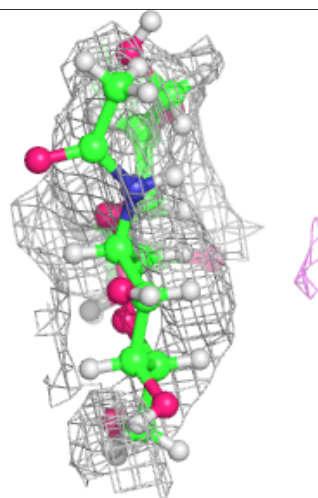
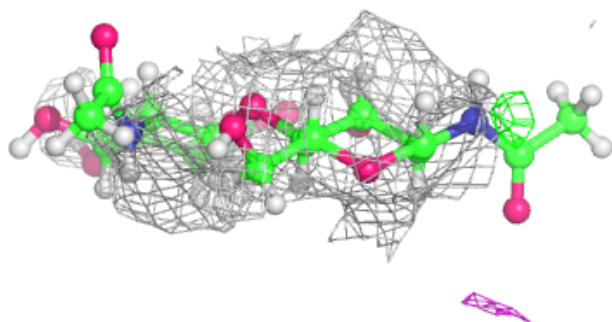
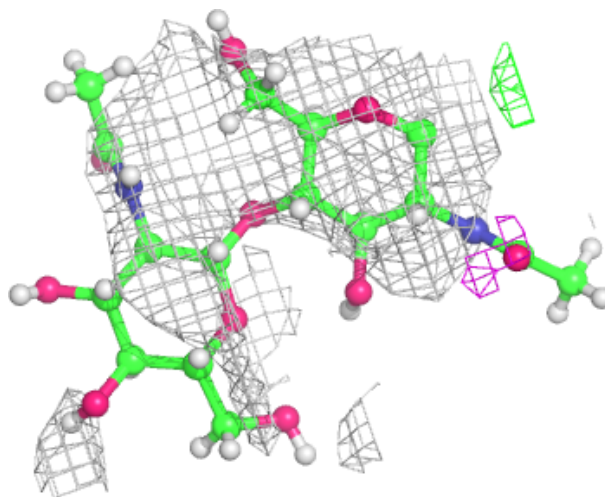
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



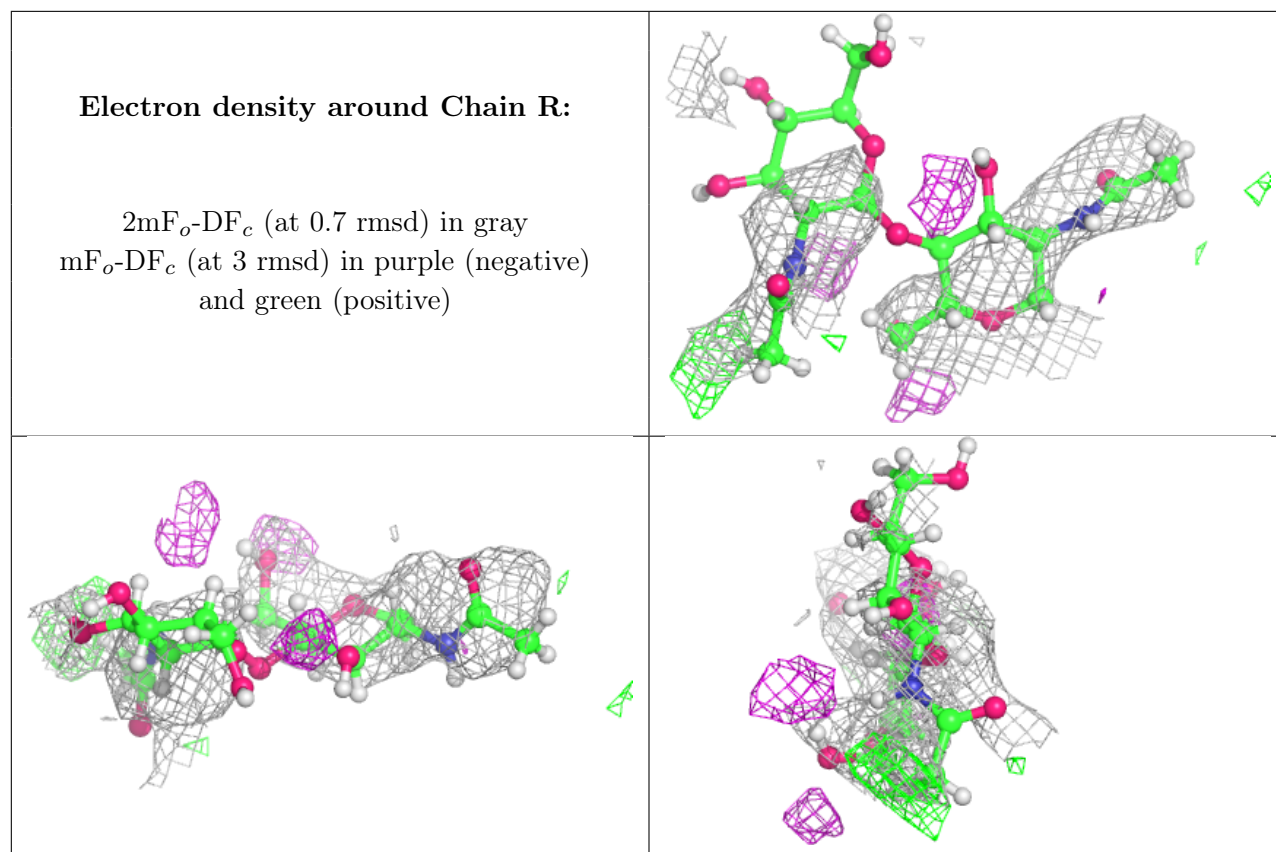


**Electron density around Chain P:**

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

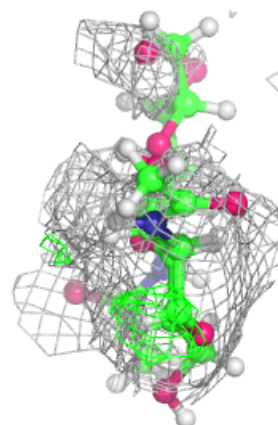
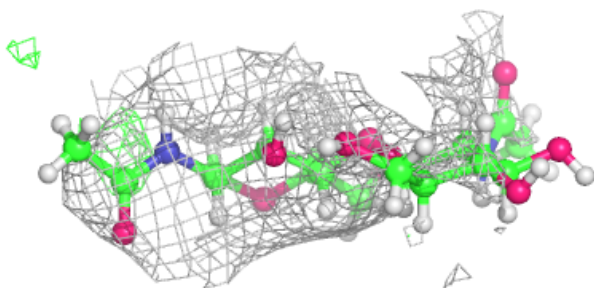
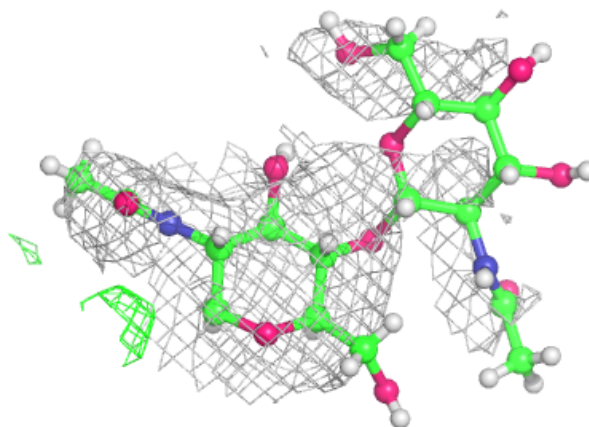






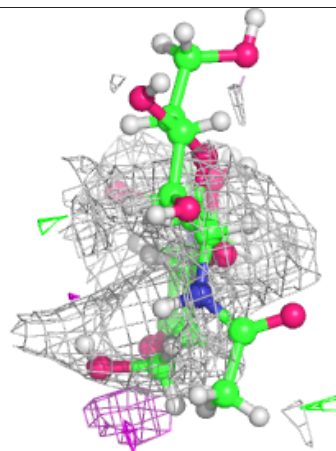
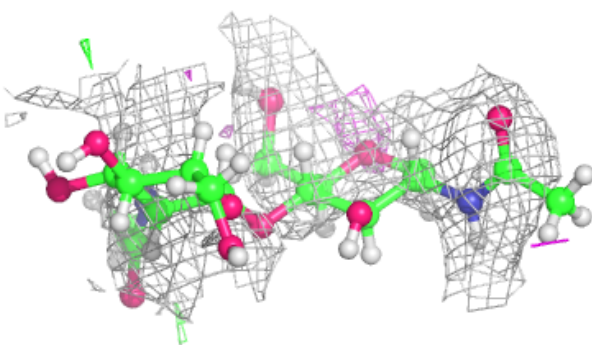
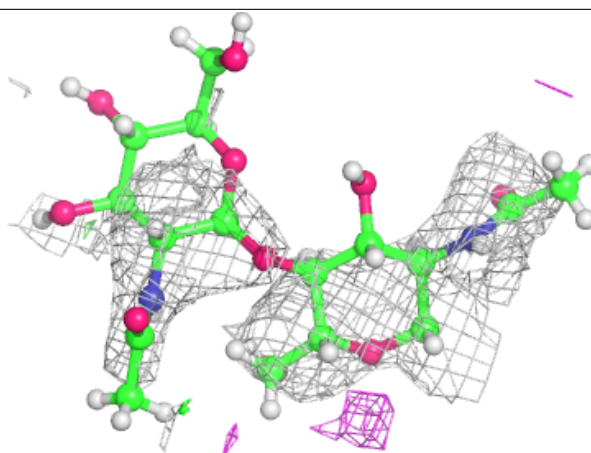
**Electron density around Chain S:**

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

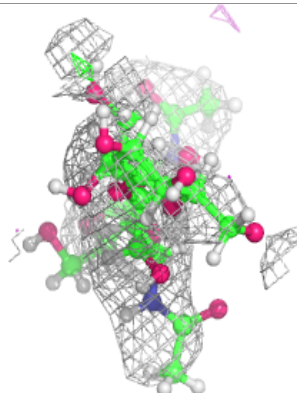
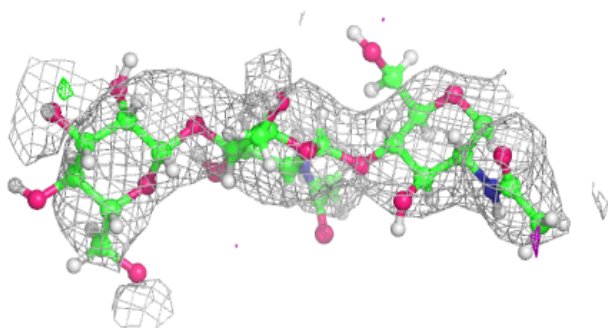
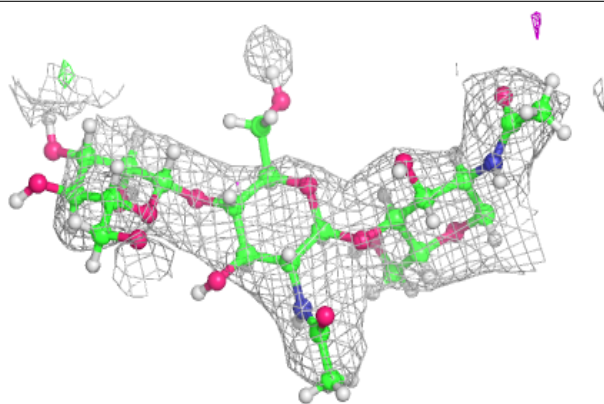


**Electron density around Chain U:**

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

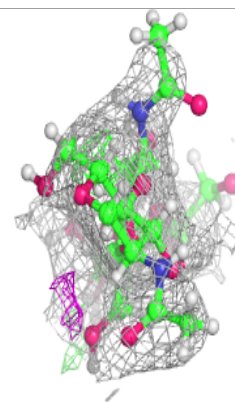
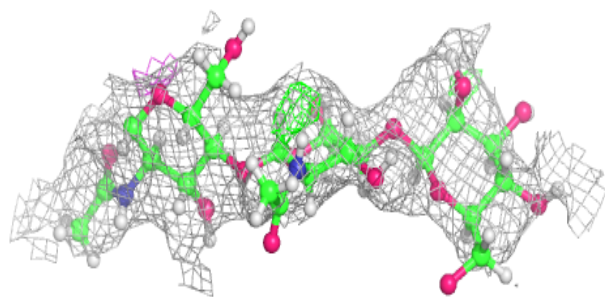
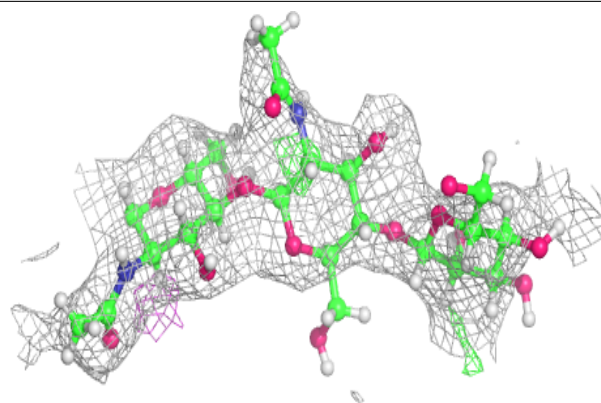
**Electron density around Chain K:**

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

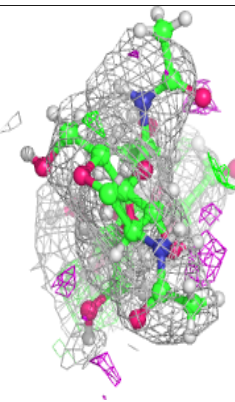
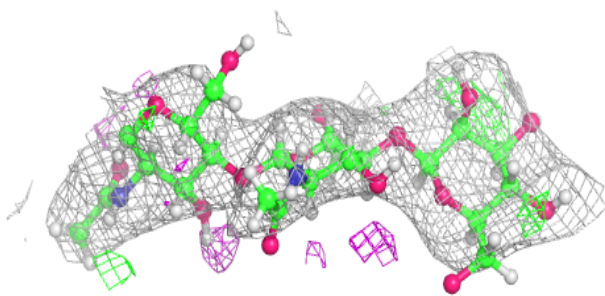
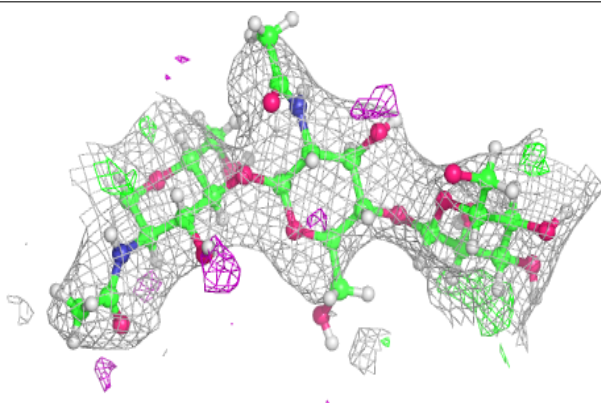


**Electron density around Chain Q:**

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

**Electron density around Chain T:**

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



## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	NAG	E	407	14/15	0.43	0.43	58,104,151,154	0
7	NAG	A	407	14/15	0.53	0.40	53,97,139,154	0
7	NAG	C	407	14/15	0.56	0.54	51,107,132,155	0
7	NAG	A	406	14/15	0.59	0.54	75,111,140,149	0
7	NAG	E	406	14/15	0.65	0.54	78,110,139,143	0
7	NAG	C	406	14/15	0.71	0.29	83,108,138,146	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.