



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:58 AM BST

PDB ID : 6V48  
Title : The crystal structure of hemagglutinin from A/mallard/Gurjev/263/1982 (H14N5)  
Authors : Yang, H.; Stevens, J.  
Deposited on : 2019-11-27  
Resolution : 3.00 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  
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

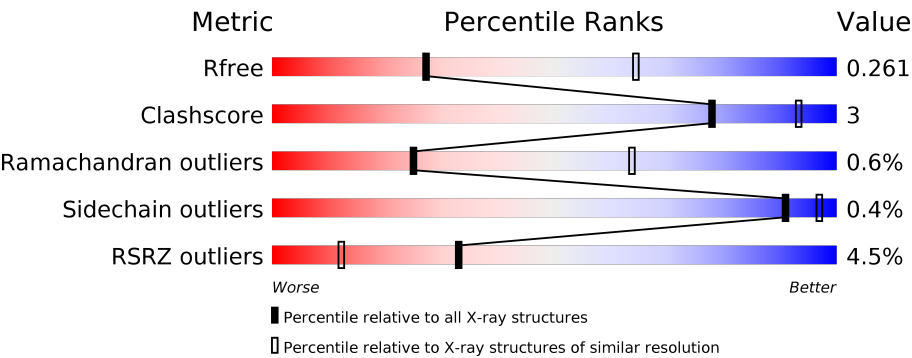
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



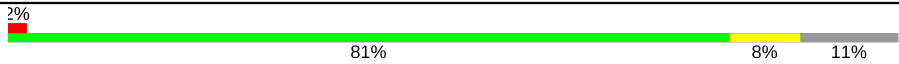













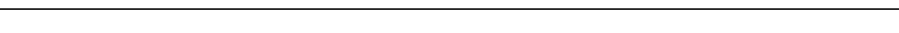

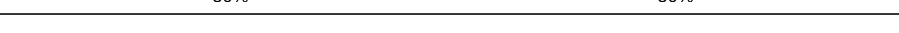
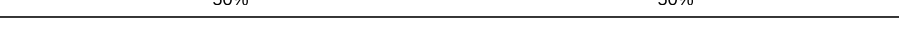
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	335	<div><div>11%</div><div>85%</div><div>10%</div><div>5%</div></div>
1	C	335	<div><div>85%</div><div>10%</div><div>5%</div></div>
1	E	335	<div><div>12%</div><div>84%</div><div>11%</div><div>5%</div></div>
1	G	335	<div><div>84%</div><div>10%</div><div>5%</div></div>
1	I	335	<div><div>86%</div><div>9%</div><div>5%</div></div>
1	K	335	<div><div>12%</div><div>84%</div><div>11%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
2	B	188	
2	D	188	
2	F	188	
2	H	188	
2	J	188	
2	L	188	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	W	2	
3	X	2	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23322 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2442	1519	436	476	11			
1	C	319	Total	C	N	O	S	0	0	0
			2442	1519	436	476	11			
1	E	319	Total	C	N	O	S	0	0	0
			2442	1519	436	476	11			
1	G	319	Total	C	N	O	S	0	0	0
			2442	1519	436	476	11			
1	I	319	Total	C	N	O	S	0	0	0
			2442	1519	436	476	11			
1	K	319	Total	C	N	O	S	0	0	0
			2442	1519	436	476	11			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP P26136
A	-2	ASP	-	expression tag	UNP P26136
A	-1	PRO	-	expression tag	UNP P26136
A	0	GLY	-	expression tag	UNP P26136
A	65	ASP	HIS	conflict	UNP P26136
C	-3	ALA	-	expression tag	UNP P26136
C	-2	ASP	-	expression tag	UNP P26136
C	-1	PRO	-	expression tag	UNP P26136
C	0	GLY	-	expression tag	UNP P26136
C	65	ASP	HIS	conflict	UNP P26136
E	-3	ALA	-	expression tag	UNP P26136
E	-2	ASP	-	expression tag	UNP P26136
E	-1	PRO	-	expression tag	UNP P26136
E	0	GLY	-	expression tag	UNP P26136
E	65	ASP	HIS	conflict	UNP P26136
G	-3	ALA	-	expression tag	UNP P26136
G	-2	ASP	-	expression tag	UNP P26136

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	PRO	-	expression tag	UNP P26136
G	0	GLY	-	expression tag	UNP P26136
G	65	ASP	HIS	conflict	UNP P26136
I	-3	ALA	-	expression tag	UNP P26136
I	-2	ASP	-	expression tag	UNP P26136
I	-1	PRO	-	expression tag	UNP P26136
I	0	GLY	-	expression tag	UNP P26136
I	65	ASP	HIS	conflict	UNP P26136
K	-3	ALA	-	expression tag	UNP P26136
K	-2	ASP	-	expression tag	UNP P26136
K	-1	PRO	-	expression tag	UNP P26136
K	0	GLY	-	expression tag	UNP P26136
K	65	ASP	HIS	conflict	UNP P26136

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	168	Total	C	N	O	S	0	0	0
			1375	849	247	275	4			
2	D	168	Total	C	N	O	S	0	0	0
			1375	849	247	275	4			
2	F	168	Total	C	N	O	S	0	0	0
			1375	849	247	275	4			
2	H	168	Total	C	N	O	S	0	0	0
			1375	849	247	275	4			
2	J	168	Total	C	N	O	S	0	0	0
			1375	849	247	275	4			
2	L	168	Total	C	N	O	S	0	0	0
			1375	849	247	275	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	182	SER	-	expression tag	UNP P26136
B	183	GLY	-	expression tag	UNP P26136
B	184	ARG	-	expression tag	UNP P26136
B	185	LEU	-	expression tag	UNP P26136
B	186	VAL	-	expression tag	UNP P26136
B	187	PRO	-	expression tag	UNP P26136
B	188	ARG	-	expression tag	UNP P26136
D	182	SER	-	expression tag	UNP P26136
D	183	GLY	-	expression tag	UNP P26136

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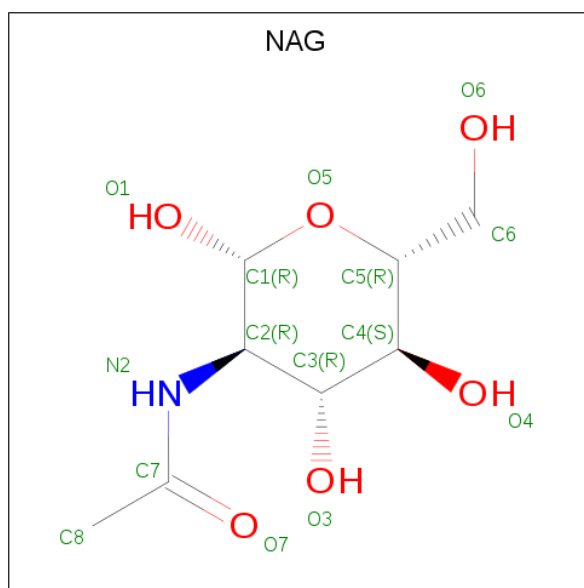
Chain	Residue	Modelled	Actual	Comment	Reference
D	184	ARG	-	expression tag	UNP P26136
D	185	LEU	-	expression tag	UNP P26136
D	186	VAL	-	expression tag	UNP P26136
D	187	PRO	-	expression tag	UNP P26136
D	188	ARG	-	expression tag	UNP P26136
F	182	SER	-	expression tag	UNP P26136
F	183	GLY	-	expression tag	UNP P26136
F	184	ARG	-	expression tag	UNP P26136
F	185	LEU	-	expression tag	UNP P26136
F	186	VAL	-	expression tag	UNP P26136
F	187	PRO	-	expression tag	UNP P26136
F	188	ARG	-	expression tag	UNP P26136
H	182	SER	-	expression tag	UNP P26136
H	183	GLY	-	expression tag	UNP P26136
H	184	ARG	-	expression tag	UNP P26136
H	185	LEU	-	expression tag	UNP P26136
H	186	VAL	-	expression tag	UNP P26136
H	187	PRO	-	expression tag	UNP P26136
H	188	ARG	-	expression tag	UNP P26136
J	182	SER	-	expression tag	UNP P26136
J	183	GLY	-	expression tag	UNP P26136
J	184	ARG	-	expression tag	UNP P26136
J	185	LEU	-	expression tag	UNP P26136
J	186	VAL	-	expression tag	UNP P26136
J	187	PRO	-	expression tag	UNP P26136
J	188	ARG	-	expression tag	UNP P26136
L	182	SER	-	expression tag	UNP P26136
L	183	GLY	-	expression tag	UNP P26136
L	184	ARG	-	expression tag	UNP P26136
L	185	LEU	-	expression tag	UNP P26136
L	186	VAL	-	expression tag	UNP P26136
L	187	PRO	-	expression tag	UNP P26136
L	188	ARG	-	expression tag	UNP P26136

- 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	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	X	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



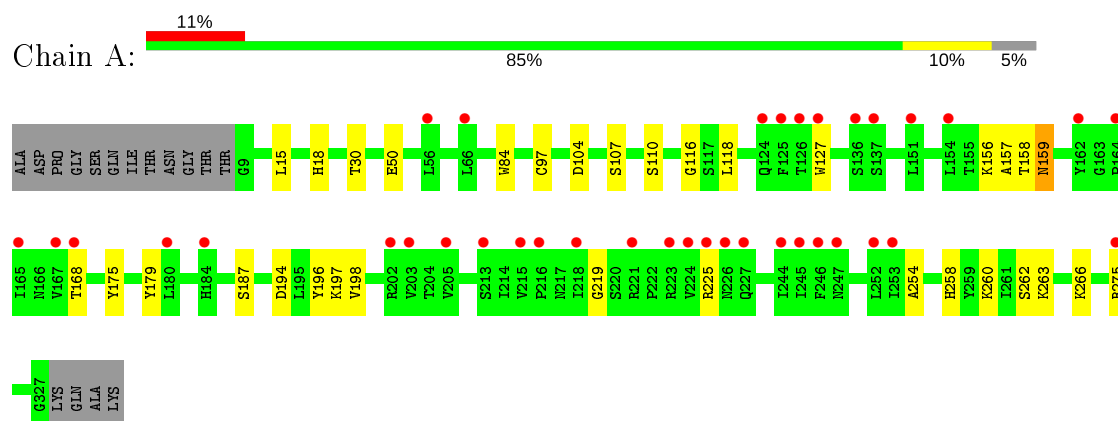
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		



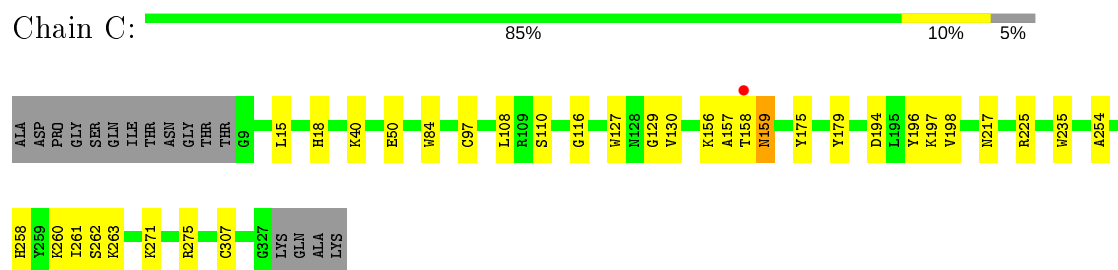
### 3 Residue-property plots [i](#)

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.

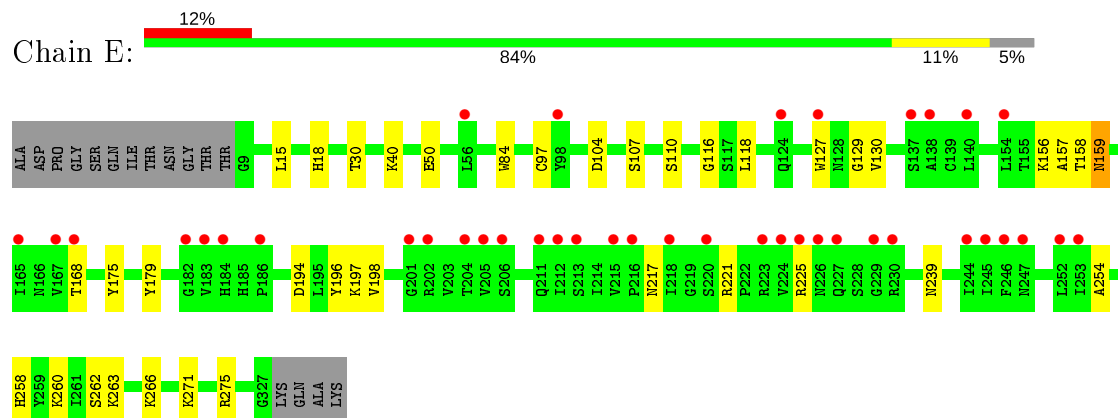
- Molecule 1: Hemagglutinin HA1 chain




- Molecule 1: Hemagglutinin HA1 chain

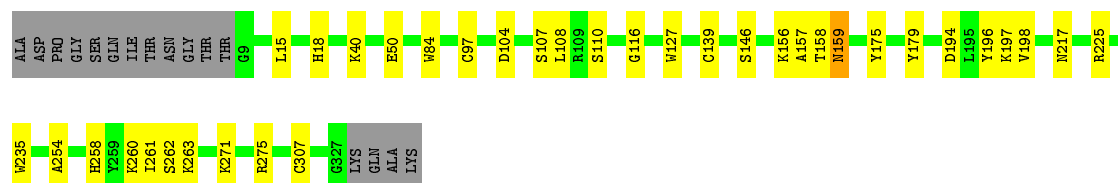


- Molecule 1: Hemagglutinin HA1 chain




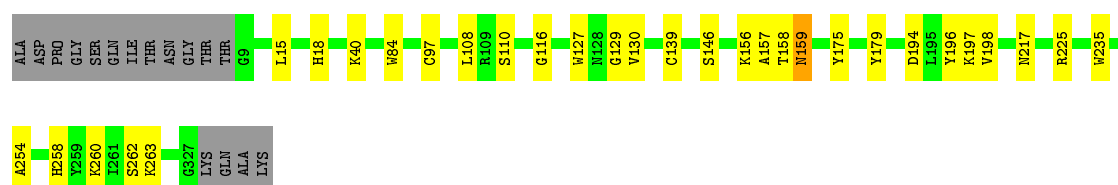
- Molecule 1: Hemagglutinin HA1 chain

Chain G: 




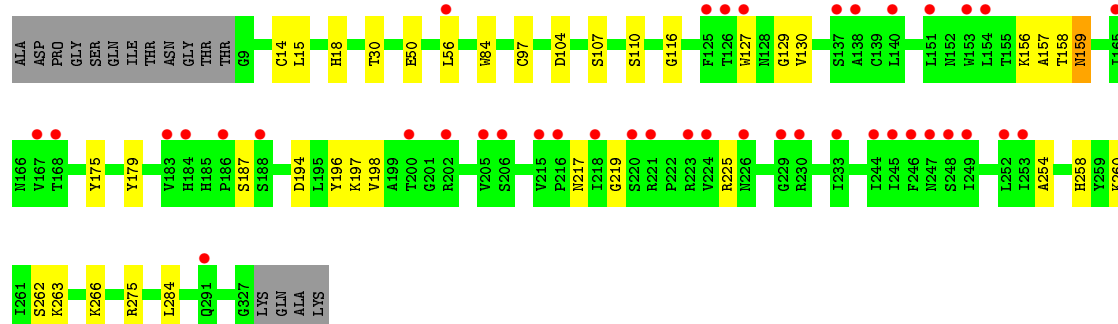
- Molecule 1: Hemagglutinin HA1 chain

Chain I: 




- Molecule 1: Hemagglutinin HA1 chain

Chain K: 




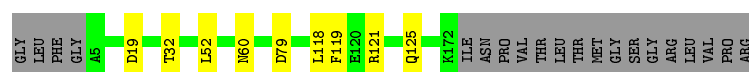
- Molecule 2: Hemagglutinin HA2 chain

Chain B: 

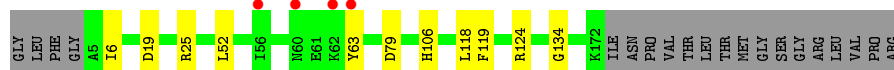
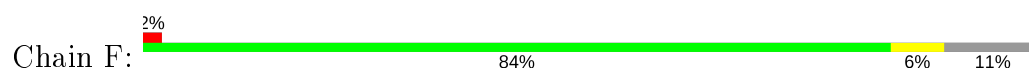


- Molecule 2: Hemagglutinin HA2 chain

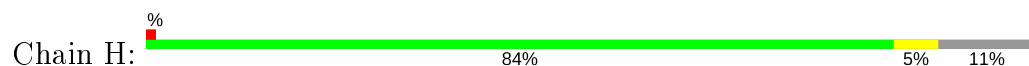
Chain D: 



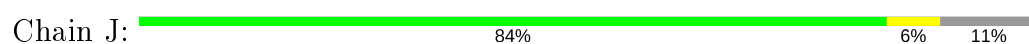
- Molecule 2: Hemagglutinin HA2 chain



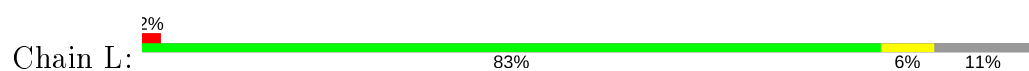
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



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



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



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



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

Chain P:  50% 50%



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

Chain Q:  50% 50%



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

Chain R:  100%



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

Chain S:  50% 50%



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

Chain T:  50% 50%



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

Chain U:  50% 50%



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

Chain V:  50% 50%



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

Chain W:  50% 50%



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

Chain X:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.66Å 100.97Å 236.07Å 90.00° 103.93° 90.00°	Depositor
Resolution (Å)	45.11 – 3.00 49.31 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.11-3.00) 97.7 (49.31-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.224 , 0.260 0.225 , 0.261	Depositor DCC
$R_{free}$ test set	3955 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 4.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.399 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.399 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0936e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0/2492	0.47	0/3387
1	C	0.26	0/2492	0.48	0/3387
1	E	0.25	0/2492	0.47	0/3387
1	G	0.26	0/2492	0.48	0/3387
1	I	0.26	0/2492	0.48	0/3387
1	K	0.25	0/2492	0.47	0/3387
2	B	0.26	0/1397	0.46	0/1882
2	D	0.27	0/1397	0.46	0/1882
2	F	0.26	0/1397	0.46	0/1882
2	H	0.27	0/1397	0.46	0/1882
2	J	0.27	0/1397	0.46	0/1882
2	L	0.26	0/1397	0.46	0/1882
All	All	0.26	0/23334	0.47	0/31614

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2442	0	2401	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2442	0	2402	18	1
1	E	2442	0	2401	23	0
1	G	2442	0	2402	19	1
1	I	2442	0	2402	15	1
1	K	2442	0	2402	20	0
2	B	1375	0	1294	12	0
2	D	1375	0	1294	7	1
2	F	1375	0	1294	10	0
2	H	1375	0	1294	7	1
2	J	1375	0	1294	7	1
2	L	1375	0	1294	11	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
4	A	14	0	13	1	0
4	C	14	0	13	0	0
4	E	14	0	13	1	0
4	G	14	0	13	0	0
4	I	14	0	13	0	0
4	K	14	0	13	0	0
All	All	23322	0	22552	135	3

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

All (135) 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:32:THR:HG22	2:D:32:THR:HG22	1.68	0.74
1:E:217:ASN:OD1	1:E:221:ARG:NH2	2.24	0.71
1:C:15:LEU:HD22	2:D:118:LEU:HG	1.77	0.67
1:G:15:LEU:HD22	2:H:118:LEU:HG	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:LEU:HD22	2:J:118:LEU:HG	1.78	0.66
1:I:157:ALA:O	1:I:159:ASN:N	2.30	0.65
1:E:97:CYS:O	1:E:225:ARG:NH1	2.31	0.64
1:E:157:ALA:O	1:E:159:ASN:N	2.31	0.64
1:C:157:ALA:O	1:C:159:ASN:N	2.31	0.63
1:K:157:ALA:O	1:K:159:ASN:N	2.31	0.63
1:A:97:CYS:O	1:A:225:ARG:NH1	2.31	0.63
1:G:157:ALA:O	1:G:159:ASN:N	2.31	0.63
1:A:157:ALA:O	1:A:159:ASN:N	2.32	0.63
1:K:97:CYS:O	1:K:225:ARG:NH1	2.32	0.62
1:E:196:TYR:O	1:E:198:VAL:N	2.33	0.61
1:A:196:TYR:O	1:A:198:VAL:N	2.32	0.61
1:I:97:CYS:O	1:I:225:ARG:NH1	2.34	0.61
1:K:196:TYR:O	1:K:198:VAL:N	2.33	0.61
1:C:196:TYR:O	1:C:198:VAL:N	2.34	0.60
1:G:196:TYR:O	1:G:198:VAL:N	2.35	0.60
1:I:196:TYR:O	1:I:198:VAL:N	2.34	0.60
1:G:97:CYS:O	1:G:225:ARG:NH1	2.35	0.59
1:E:15:LEU:HD22	2:F:118:LEU:HG	1.84	0.59
1:G:15:LEU:HD13	2:H:119:PHE:HA	1.83	0.59
1:C:15:LEU:HD13	2:D:119:PHE:HA	1.84	0.59
1:A:15:LEU:HD22	2:B:118:LEU:HG	1.86	0.58
2:B:134:GLY:HA2	2:F:124:ARG:HD3	1.86	0.58
1:A:110:SER:OG	2:L:79:ASP:OD2	2.20	0.58
2:B:79:ASP:OD2	1:E:110:SER:OG	2.21	0.57
1:K:15:LEU:HD22	2:L:118:LEU:HG	1.86	0.57
2:B:19:ASP:N	2:B:19:ASP:OD1	2.39	0.56
1:C:97:CYS:O	1:C:225:ARG:NH1	2.39	0.56
2:L:19:ASP:OD1	2:L:19:ASP:N	2.39	0.56
2:F:134:GLY:HA2	2:L:124:ARG:HD3	1.88	0.56
1:A:168:THR:HG21	4:A:501:NAG:H81	1.87	0.55
2:J:19:ASP:N	2:J:19:ASP:OD1	2.41	0.55
2:F:79:ASP:OD2	1:K:110:SER:OG	2.22	0.54
1:I:15:LEU:HD13	2:J:119:PHE:HA	1.90	0.54
2:F:19:ASP:OD1	2:F:19:ASP:N	2.39	0.54
1:A:175:TYR:CD1	1:A:260:LYS:HG3	2.44	0.53
2:D:19:ASP:OD1	2:D:19:ASP:N	2.41	0.53
2:H:19:ASP:OD1	2:H:19:ASP:N	2.40	0.53
1:E:175:TYR:CD1	1:E:260:LYS:HG3	2.45	0.52
1:K:175:TYR:CD1	1:K:260:LYS:HG3	2.45	0.51
1:E:30:THR:HG21	2:L:106:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:ARG:HD3	2:L:134:GLY:HA2	1.92	0.50
1:K:104:ASP:HB3	1:K:107:SER:HB2	1.93	0.50
1:C:175:TYR:CD1	1:C:260:LYS:HG3	2.47	0.50
1:I:84:TRP:CE2	1:I:116:GLY:HA2	2.47	0.49
1:G:175:TYR:CD1	1:G:260:LYS:HG3	2.47	0.49
1:E:262:SER:O	1:E:263:LYS:HB3	2.13	0.49
1:I:179:TYR:CE2	1:I:258:HIS:HB3	2.48	0.48
1:A:30:THR:HG21	2:F:106:HIS:CE1	2.48	0.48
1:I:40:LYS:HD3	2:J:52:LEU:HD11	1.96	0.48
2:B:106:HIS:CE1	1:K:30:THR:HG21	2.48	0.48
1:E:104:ASP:HB3	1:E:107:SER:HB2	1.96	0.48
1:G:262:SER:O	1:G:263:LYS:HB3	2.14	0.48
1:A:179:TYR:CE2	1:A:258:HIS:HB3	2.49	0.48
1:A:104:ASP:HB3	1:A:107:SER:HB2	1.96	0.48
1:I:175:TYR:CD1	1:I:260:LYS:HG3	2.49	0.47
1:E:179:TYR:CE2	1:E:258:HIS:HB3	2.50	0.47
1:K:262:SER:O	1:K:263:LYS:HB3	2.14	0.47
1:K:127:TRP:CZ2	1:K:254:ALA:HB1	2.49	0.47
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.49	0.47
1:C:179:TYR:CE2	1:C:258:HIS:HB3	2.49	0.47
1:K:179:TYR:CE2	1:K:258:HIS:HB3	2.49	0.47
1:A:262:SER:O	1:A:263:LYS:HB3	2.14	0.47
1:C:156:LYS:HD3	1:C:194:ASP:O	2.15	0.47
1:E:168:THR:HG21	4:E:501:NAG:H81	1.96	0.47
1:A:127:TRP:CZ2	1:A:254:ALA:HB1	2.50	0.47
1:G:156:LYS:HD3	1:G:194:ASP:O	2.15	0.47
1:C:262:SER:O	1:C:263:LYS:HB3	2.15	0.47
1:I:262:SER:O	1:I:263:LYS:HB3	2.15	0.47
1:I:156:LYS:HD3	1:I:194:ASP:O	2.15	0.46
1:G:127:TRP:CZ2	1:G:254:ALA:HB1	2.51	0.46
1:E:127:TRP:CZ2	1:E:254:ALA:HB1	2.50	0.45
1:C:50:GLU:OE2	1:C:275:ARG:NH2	2.49	0.45
1:G:179:TYR:CE2	1:G:258:HIS:HB3	2.52	0.45
2:D:121:ARG:O	2:D:125:GLN:HG3	2.16	0.45
1:E:156:LYS:HD3	1:E:194:ASP:O	2.17	0.45
1:G:40:LYS:HD3	2:H:52:LEU:HD11	1.97	0.45
2:H:121:ARG:O	2:H:125:GLN:HG3	2.16	0.45
2:L:6:ILE:HD13	2:L:25:ARG:HG2	1.99	0.45
2:B:72:GLN:NE2	1:E:239:ASN:OD1	2.47	0.45
1:G:84:TRP:CE2	1:G:116:GLY:HA2	2.51	0.45
1:A:156:LYS:HD3	1:A:194:ASP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:TRP:CZ2	1:C:254:ALA:HB1	2.52	0.45
1:E:84:TRP:CE2	1:E:116:GLY:HA2	2.52	0.45
2:L:127:ARG:HB3	2:L:128:GLU:H	1.60	0.44
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.52	0.44
2:J:121:ARG:O	2:J:125:GLN:HG3	2.17	0.44
1:I:127:TRP:CZ2	1:I:254:ALA:HB1	2.53	0.44
1:C:108:LEU:HB2	1:C:235:TRP:CZ3	2.53	0.44
2:B:121:ARG:O	2:B:125:GLN:HG3	2.18	0.44
1:E:15:LEU:HD13	2:F:119:PHE:HA	1.99	0.44
1:K:156:LYS:HD3	1:K:194:ASP:O	2.17	0.44
1:G:307:CYS:O	2:H:60:ASN:ND2	2.35	0.43
1:K:84:TRP:CE2	1:K:116:GLY:HA2	2.53	0.43
1:C:40:LYS:HD3	2:D:52:LEU:HD11	2.00	0.43
1:E:50:GLU:OE2	1:E:275:ARG:NH2	2.50	0.42
1:A:15:LEU:HD13	2:B:119:PHE:HA	2.01	0.42
2:F:6:ILE:HD13	2:F:25:ARG:HG2	2.01	0.42
1:C:271:LYS:HB2	1:C:271:LYS:HE3	1.85	0.42
1:G:50:GLU:OE2	1:G:275:ARG:NH2	2.50	0.42
1:K:129:GLY:O	1:K:130:VAL:HG13	2.20	0.42
1:E:266:LYS:O	2:F:63:TYR:HB3	2.19	0.42
2:B:6:ILE:HD13	2:B:25:ARG:HG2	2.00	0.42
1:K:15:LEU:HD13	2:L:119:PHE:HA	2.02	0.42
1:K:266:LYS:O	2:L:63:TYR:HB3	2.19	0.42
1:E:40:LYS:HD3	2:F:52:LEU:HD11	2.02	0.41
1:I:139:CYS:HB3	1:I:146:SER:O	2.20	0.41
1:G:271:LYS:HB2	1:G:271:LYS:HE3	1.86	0.41
1:A:50:GLU:OE2	1:A:275:ARG:NH2	2.50	0.41
1:C:307:CYS:O	2:D:60:ASN:ND2	2.40	0.41
1:I:108:LEU:HB2	1:I:235:TRP:CZ3	2.56	0.41
1:C:129:GLY:O	1:C:130:VAL:HG13	2.21	0.41
1:K:56:LEU:HD12	1:K:284:LEU:HG	2.02	0.41
1:K:187:SER:HA	1:K:219:GLY:O	2.21	0.41
1:E:129:GLY:O	1:E:130:VAL:HG13	2.21	0.41
2:J:74:GLU:HG3	2:J:78:GLN:NE2	2.35	0.41
1:E:271:LYS:HE3	1:E:271:LYS:HB2	1.82	0.40
2:J:127:ARG:HB3	2:J:128:GLU:H	1.65	0.40
1:K:50:GLU:OE2	1:K:275:ARG:NH2	2.53	0.40
1:A:187:SER:HA	1:A:219:GLY:O	2.21	0.40
1:C:261:ILE:HA	1:C:261:ILE:HD13	1.90	0.40
1:A:266:LYS:O	2:B:63:TYR:HB3	2.21	0.40
1:G:261:ILE:HD13	1:G:261:ILE:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:ILE:HD13	2:H:25:ARG:HG2	2.03	0.40
1:I:129:GLY:O	1:I:130:VAL:HG13	2.22	0.40
1:G:108:LEU:HB2	1:G:235:TRP:CZ3	2.56	0.40
1:K:14:CYS:SG	2:L:6:ILE:HG22	2.61	0.40
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.91	0.40
1:E:118:LEU:HD23	1:E:118:LEU:HA	1.91	0.40
1:G:104:ASP:HB3	1:G:107:SER:HB2	2.04	0.40
1:G:139:CYS:HB3	1:G:146:SER:O	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:ASP:OD2	1:G:110:SER:OG[4_545]	2.17	0.03
2:H:79:ASP:OD2	1:I:110:SER:OG[1_565]	2.17	0.03
1:C:110:SER:OG	2:J:79:ASP:OD2[4_555]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	317/335 (95%)	291 (92%)	23 (7%)	3 (1%)	17	55
1	C	317/335 (95%)	289 (91%)	25 (8%)	3 (1%)	17	55
1	E	317/335 (95%)	291 (92%)	23 (7%)	3 (1%)	17	55
1	G	317/335 (95%)	290 (92%)	24 (8%)	3 (1%)	17	55
1	I	317/335 (95%)	290 (92%)	24 (8%)	3 (1%)	17	55
1	K	317/335 (95%)	291 (92%)	23 (7%)	3 (1%)	17	55
2	B	166/188 (88%)	157 (95%)	9 (5%)	0	100	100
2	D	166/188 (88%)	157 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	166/188 (88%)	157 (95%)	9 (5%)	0	100	100
2	H	166/188 (88%)	157 (95%)	9 (5%)	0	100	100
2	J	166/188 (88%)	157 (95%)	9 (5%)	0	100	100
2	L	166/188 (88%)	157 (95%)	9 (5%)	0	100	100
All	All	2898/3138 (92%)	2684 (93%)	196 (7%)	18 (1%)	25	64

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	THR
1	A	159	ASN
1	A	197	LYS
1	C	158	THR
1	C	159	ASN
1	C	197	LYS
1	E	158	THR
1	E	159	ASN
1	E	197	LYS
1	G	158	THR
1	G	159	ASN
1	G	197	LYS
1	I	158	THR
1	I	159	ASN
1	I	197	LYS
1	K	158	THR
1	K	159	ASN
1	K	197	LYS

### 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	279/291 (96%)	278 (100%)	1 (0%)	91	97
1	C	279/291 (96%)	277 (99%)	2 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	279/291 (96%)	278 (100%)	1 (0%)	91	97
1	G	279/291 (96%)	277 (99%)	2 (1%)	84	94
1	I	279/291 (96%)	277 (99%)	2 (1%)	84	94
1	K	279/291 (96%)	277 (99%)	2 (1%)	84	94
2	B	145/161 (90%)	144 (99%)	1 (1%)	84	94
2	D	145/161 (90%)	145 (100%)	0	100	100
2	F	145/161 (90%)	145 (100%)	0	100	100
2	H	145/161 (90%)	145 (100%)	0	100	100
2	J	145/161 (90%)	145 (100%)	0	100	100
2	L	145/161 (90%)	145 (100%)	0	100	100
All	All	2544/2712 (94%)	2533 (100%)	11 (0%)	91	97

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
2	B	143	GLN
1	C	18	HIS
1	C	217	ASN
1	E	18	HIS
1	G	18	HIS
1	G	217	ASN
1	I	18	HIS
1	I	217	ASN
1	K	18	HIS
1	K	217	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	72	GLN
1	E	239	ASN

### 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 ⓘ

24 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
3	NAG	M	1	1,3	14,14,15	0.61	0	17,19,21	0.53	0
3	NAG	M	2	3	14,14,15	1.19	1 (7%)	17,19,21	1.55	2 (11%)
3	NAG	N	1	3,2	14,14,15	0.77	1 (7%)	17,19,21	0.61	0
3	NAG	N	2	3	14,14,15	0.80	1 (7%)	17,19,21	0.43	0
3	NAG	O	1	1,3	14,14,15	0.62	0	17,19,21	0.58	0
3	NAG	O	2	3	14,14,15	0.83	1 (7%)	17,19,21	0.78	0
3	NAG	P	1	3,2	14,14,15	0.66	1 (7%)	17,19,21	0.70	0
3	NAG	P	2	3	14,14,15	0.64	0	17,19,21	0.47	0
3	NAG	Q	1	1,3	14,14,15	0.57	0	17,19,21	0.50	0
3	NAG	Q	2	3	14,14,15	1.00	1 (7%)	17,19,21	0.88	1 (5%)
3	NAG	R	1	3,2	14,14,15	0.82	1 (7%)	17,19,21	0.70	0
3	NAG	R	2	3	14,14,15	0.71	1 (7%)	17,19,21	0.43	0
3	NAG	S	1	1,3	14,14,15	0.62	0	17,19,21	0.56	0
3	NAG	S	2	3	14,14,15	0.92	1 (7%)	17,19,21	0.72	0
3	NAG	T	1	3,2	14,14,15	0.72	1 (7%)	17,19,21	0.69	0
3	NAG	T	2	3	14,14,15	0.67	0	17,19,21	0.46	0
3	NAG	U	1	1,3	14,14,15	0.55	0	17,19,21	0.56	0
3	NAG	U	2	3	14,14,15	0.87	1 (7%)	17,19,21	0.79	1 (5%)
3	NAG	V	1	3,2	14,14,15	0.70	1 (7%)	17,19,21	0.71	0
3	NAG	V	2	3	14,14,15	0.76	0	17,19,21	0.44	0
3	NAG	W	1	1,3	14,14,15	0.62	0	17,19,21	0.55	0
3	NAG	W	2	3	14,14,15	1.09	1 (7%)	17,19,21	0.88	1 (5%)
3	NAG	X	1	3,2	14,14,15	0.76	1 (7%)	17,19,21	0.71	0
3	NAG	X	2	3	14,14,15	0.84	1 (7%)	17,19,21	0.43	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
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	NAG	V	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	NAG	X	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	2	NAG	O5-C1	-4.25	1.36	1.43
3	W	2	NAG	O5-C1	-3.80	1.37	1.43
3	Q	2	NAG	O5-C1	-3.36	1.38	1.43
3	S	2	NAG	O5-C1	-3.09	1.38	1.43
3	U	2	NAG	O5-C1	-2.77	1.39	1.43
3	O	2	NAG	O5-C1	-2.74	1.39	1.43
3	R	1	NAG	C1-C2	2.71	1.56	1.52
3	N	1	NAG	C1-C2	2.51	1.56	1.52
3	X	1	NAG	C1-C2	2.46	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	2	NAG	C1-C2	2.40	1.55	1.52
3	N	2	NAG	C1-C2	2.37	1.55	1.52
3	T	1	NAG	C1-C2	2.23	1.55	1.52
3	V	1	NAG	C1-C2	2.22	1.55	1.52
3	P	1	NAG	C1-C2	2.11	1.55	1.52
3	R	2	NAG	C1-C2	2.06	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	2	NAG	C3-C4-C5	4.03	117.42	110.24
3	M	2	NAG	C4-C3-C2	3.88	116.71	111.02
3	W	2	NAG	C4-C3-C2	2.37	114.49	111.02
3	Q	2	NAG	C4-C3-C2	2.29	114.37	111.02
3	U	2	NAG	C4-C3-C2	2.15	114.17	111.02

There are no chirality outliers.

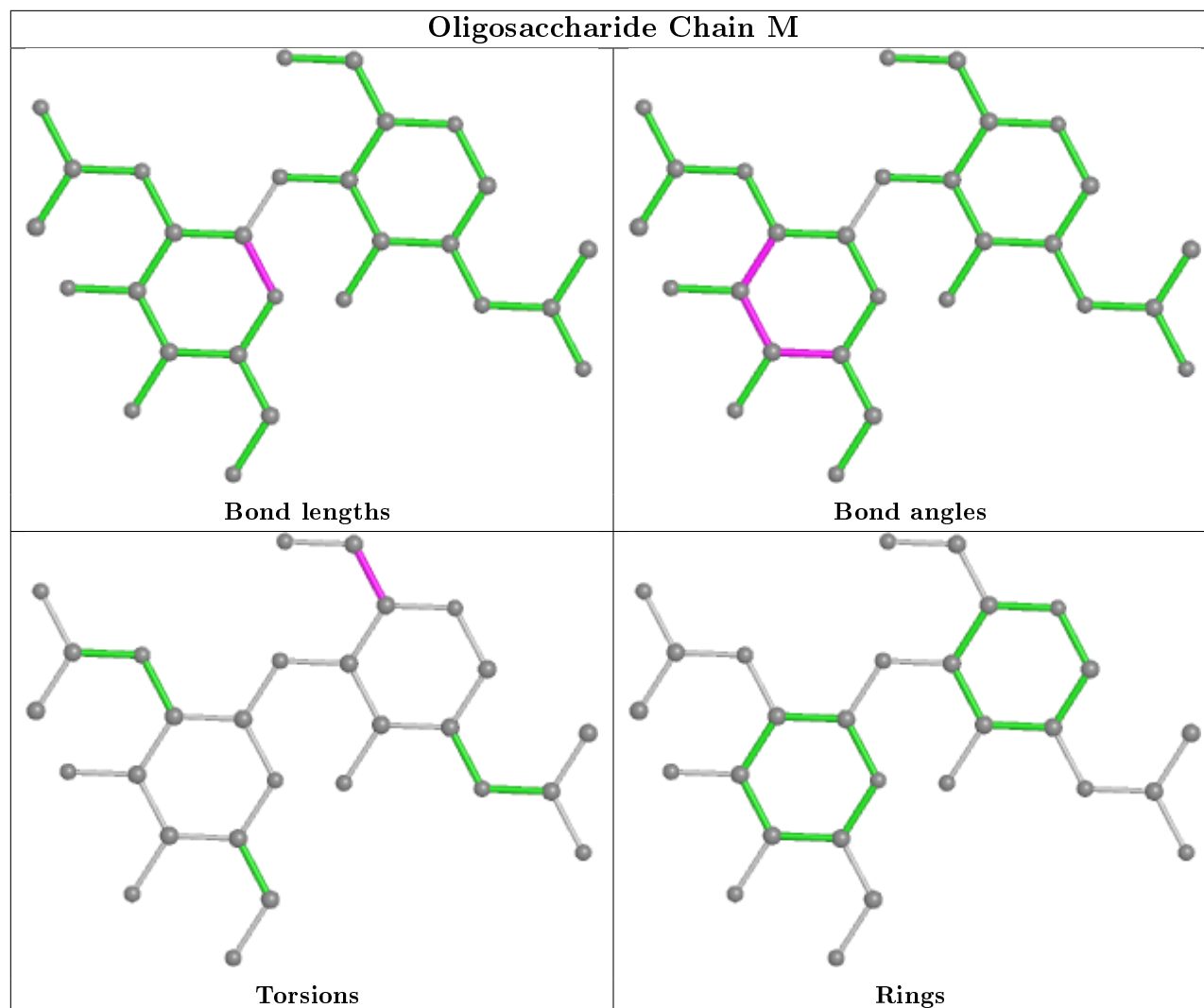
All (16) torsion outliers are listed below:

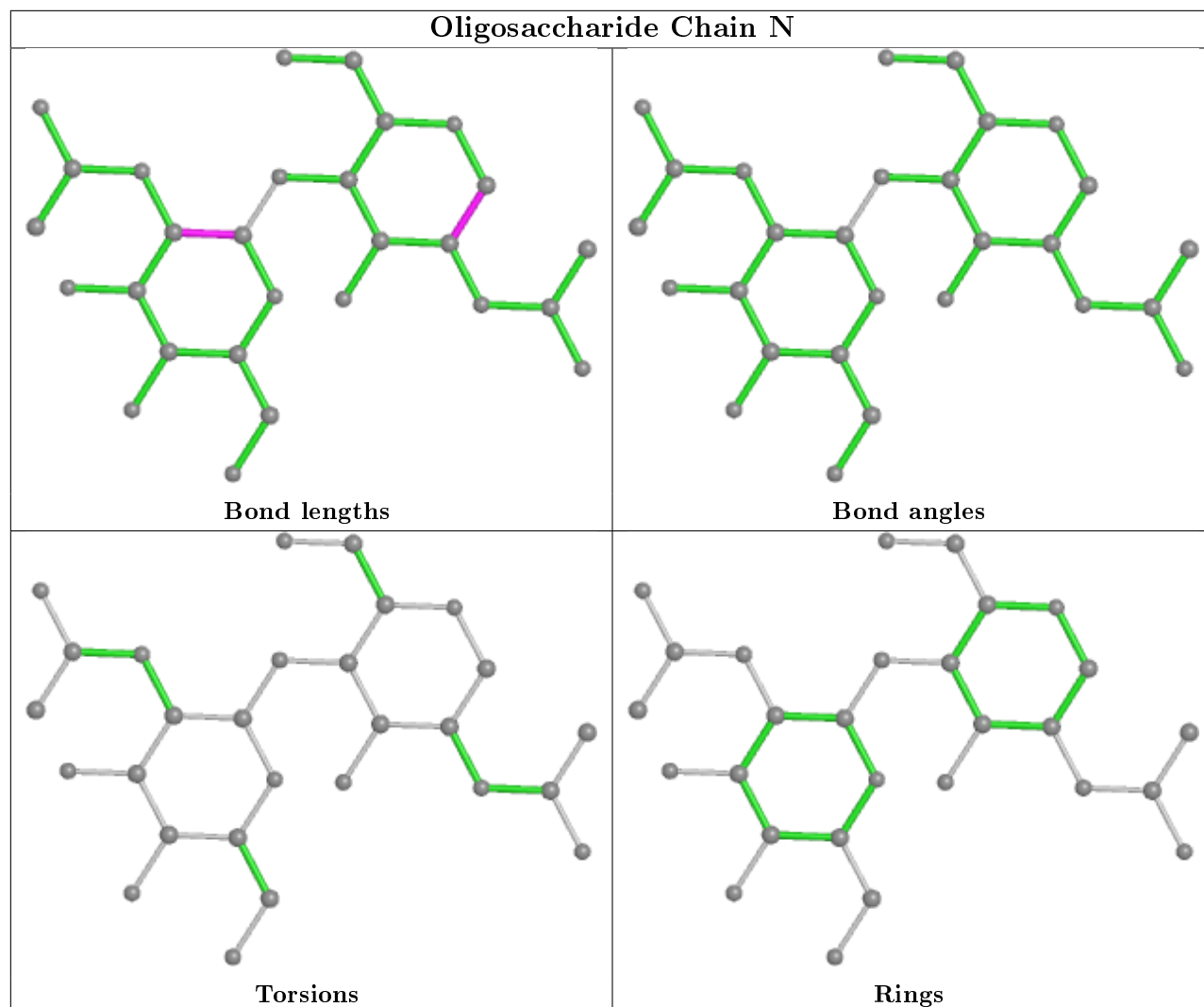
Mol	Chain	Res	Type	Atoms
3	R	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6

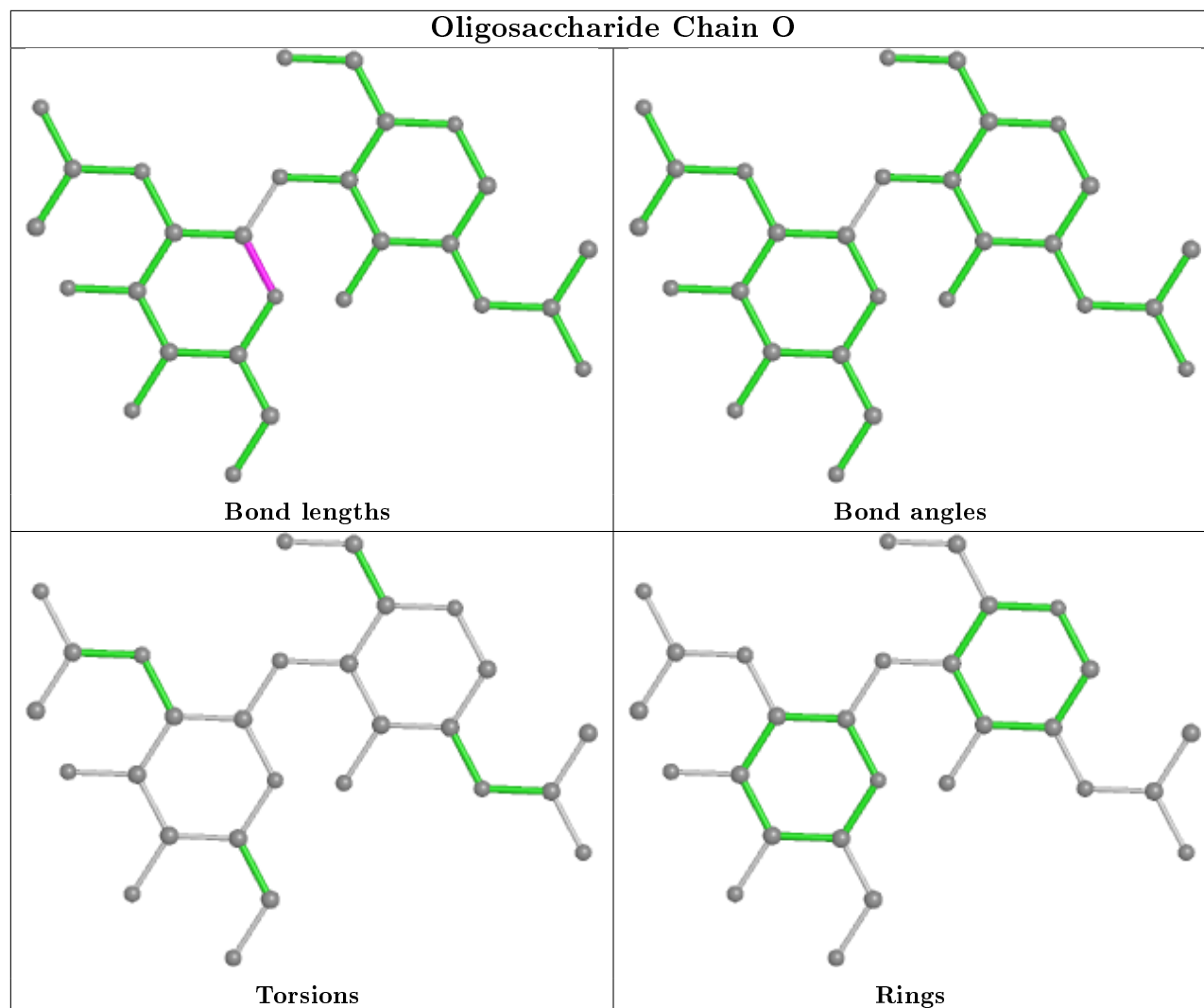
There are no ring outliers.

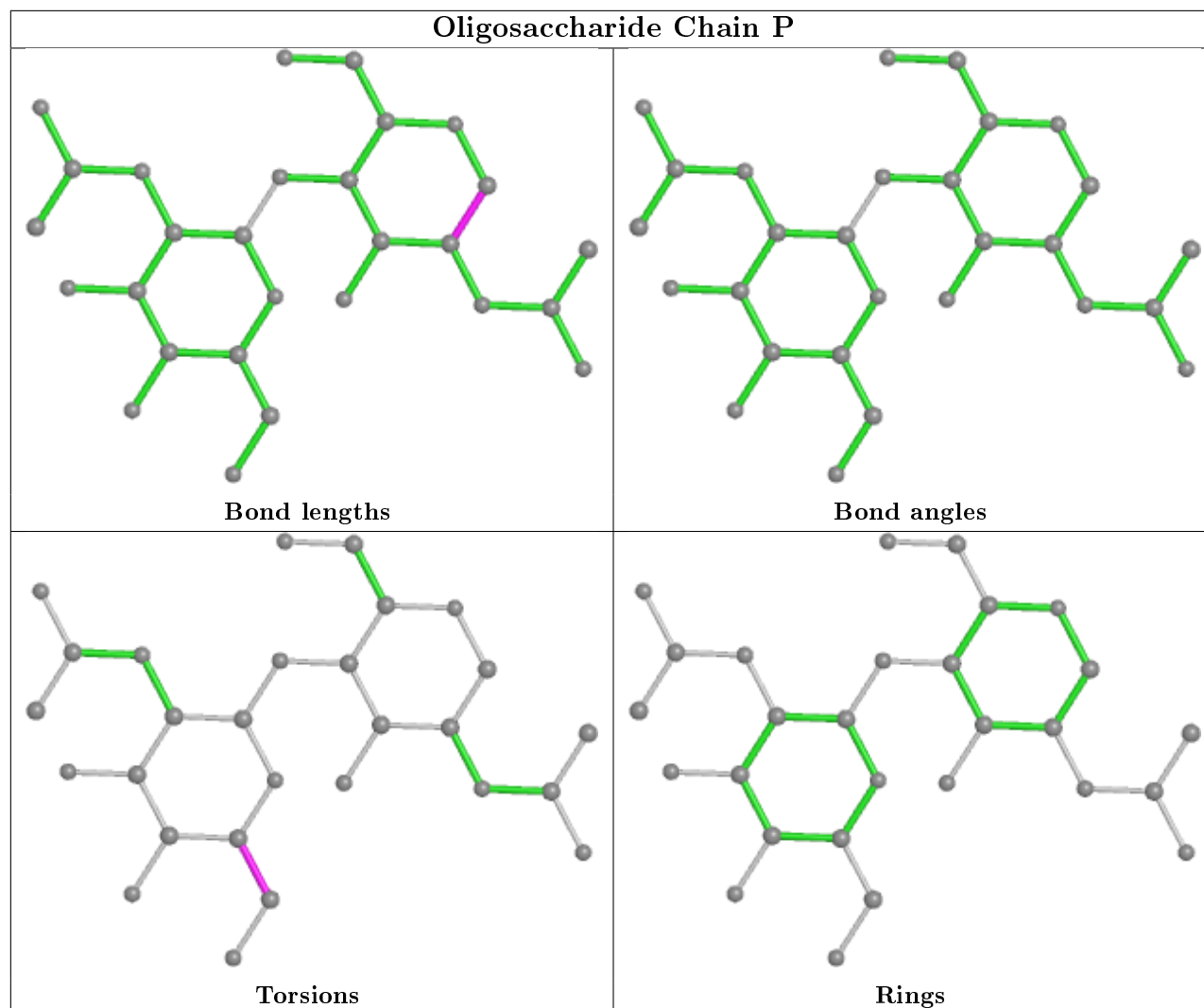
No monomer is involved in short contacts.

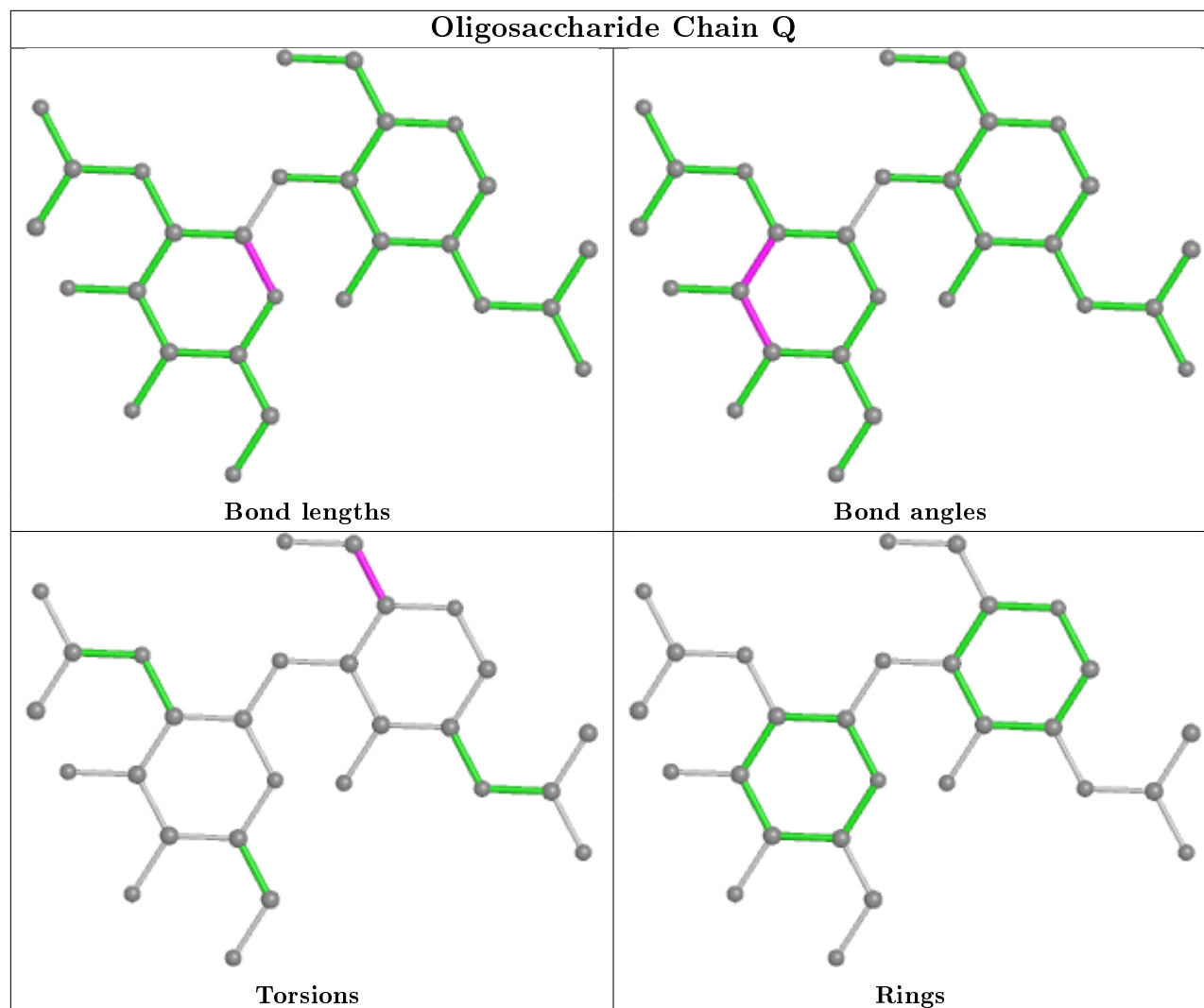
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

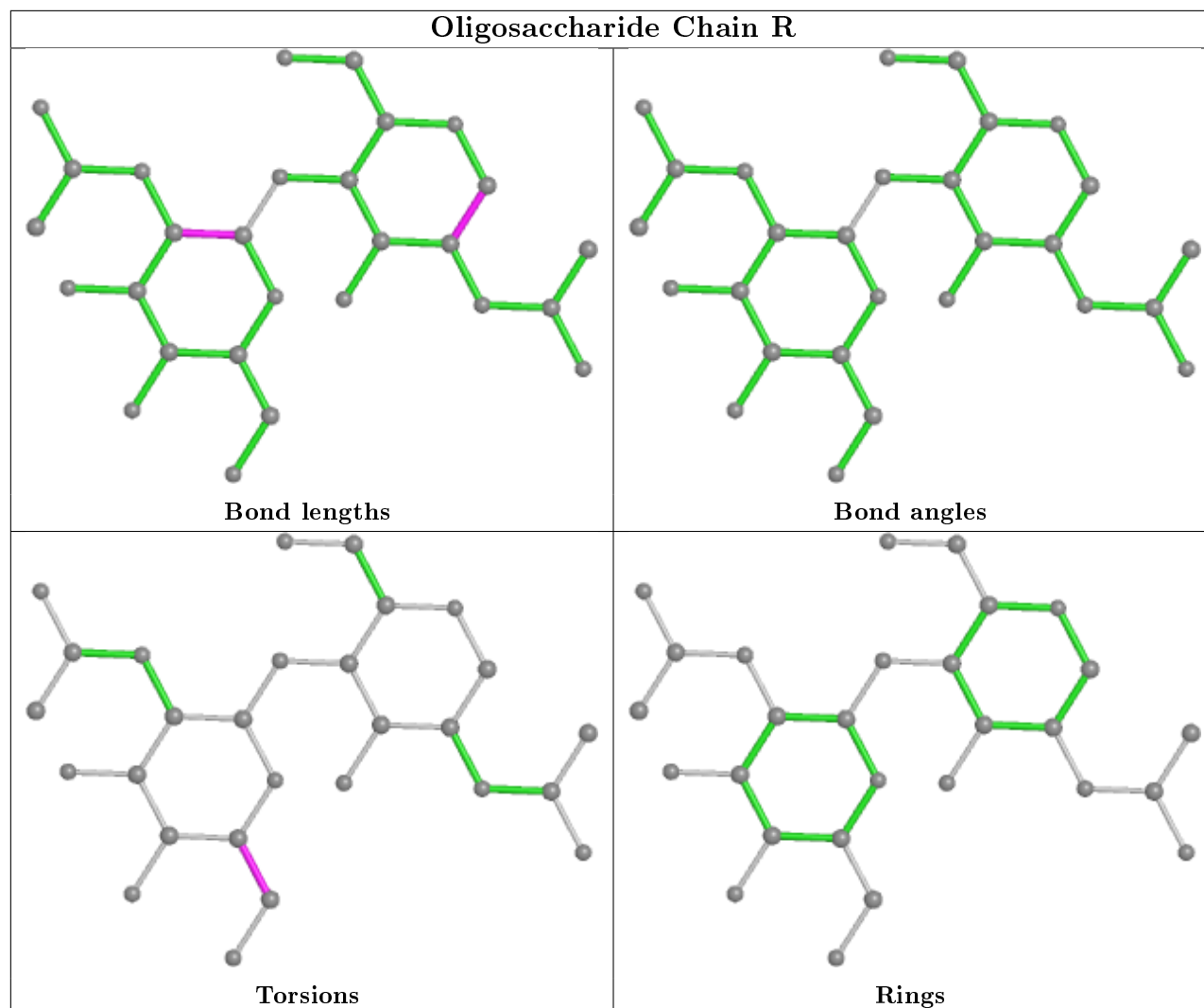


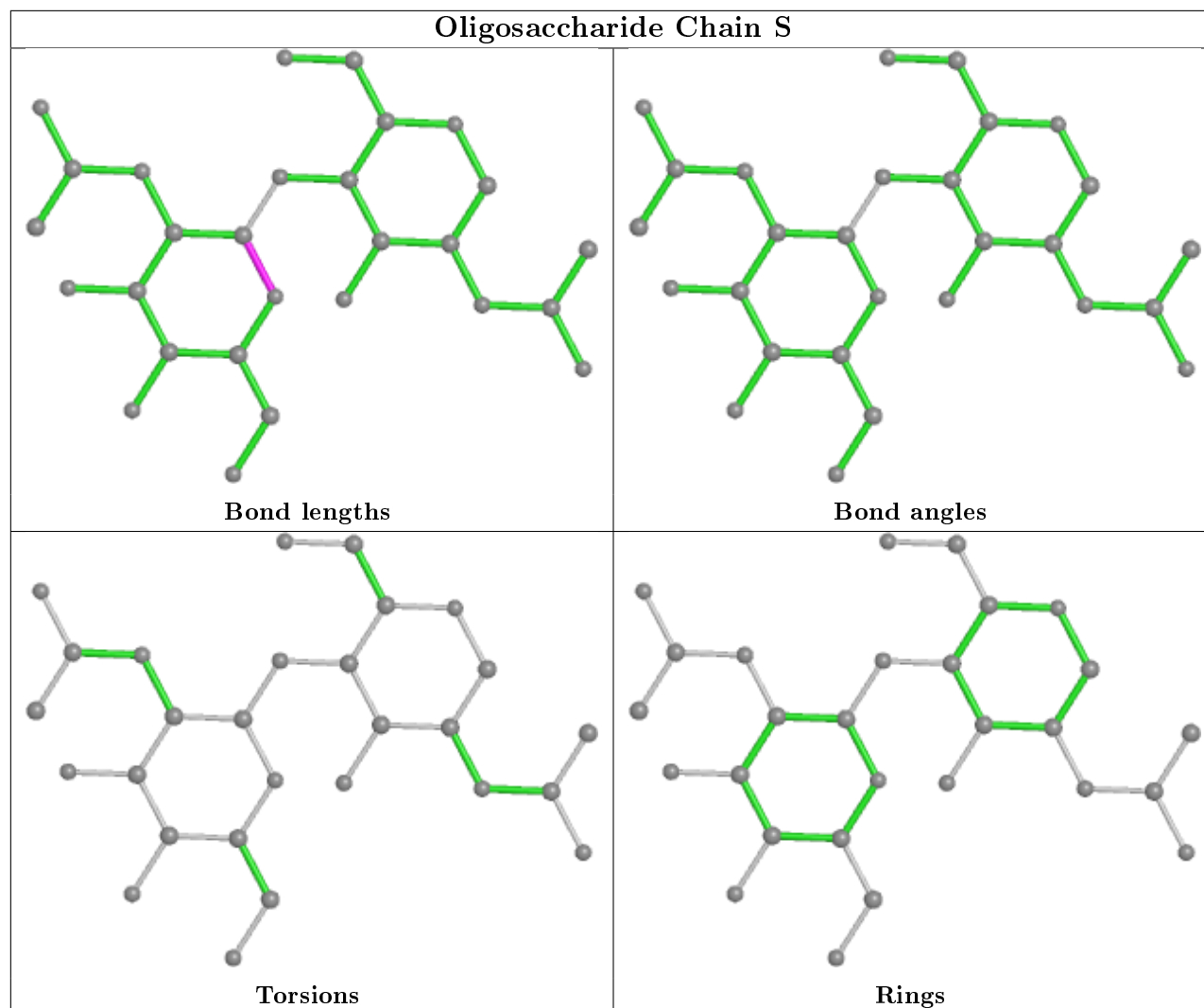




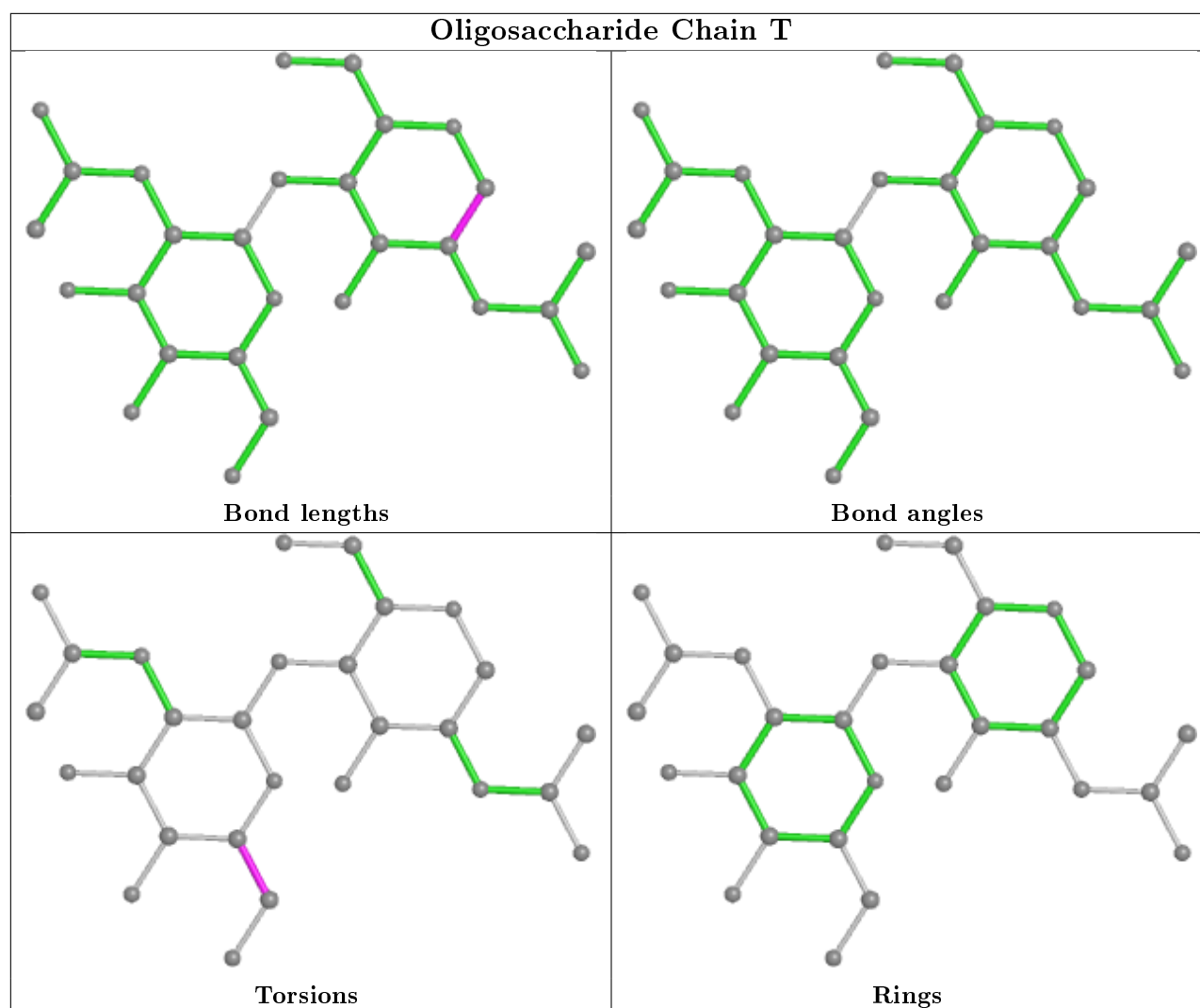


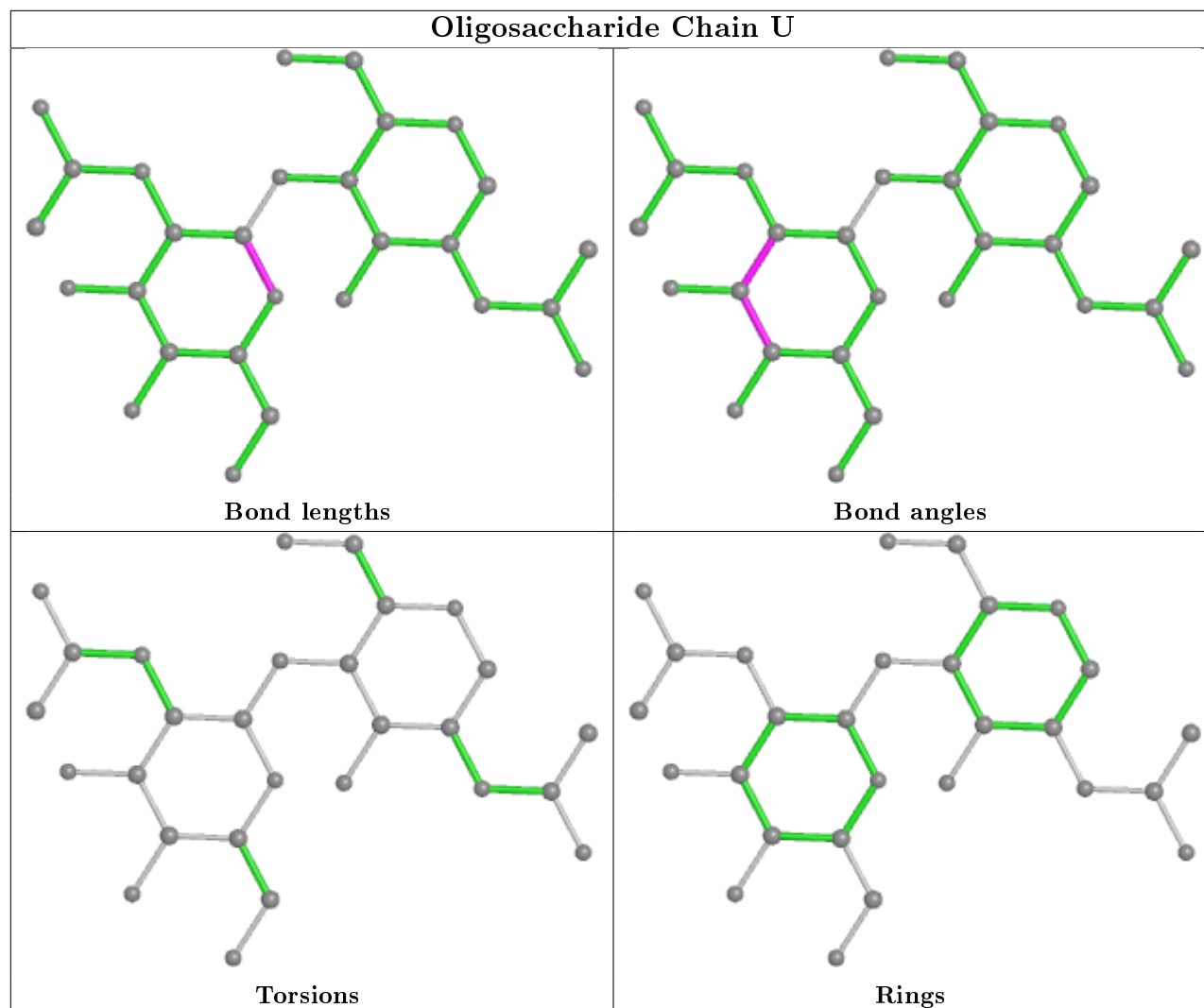


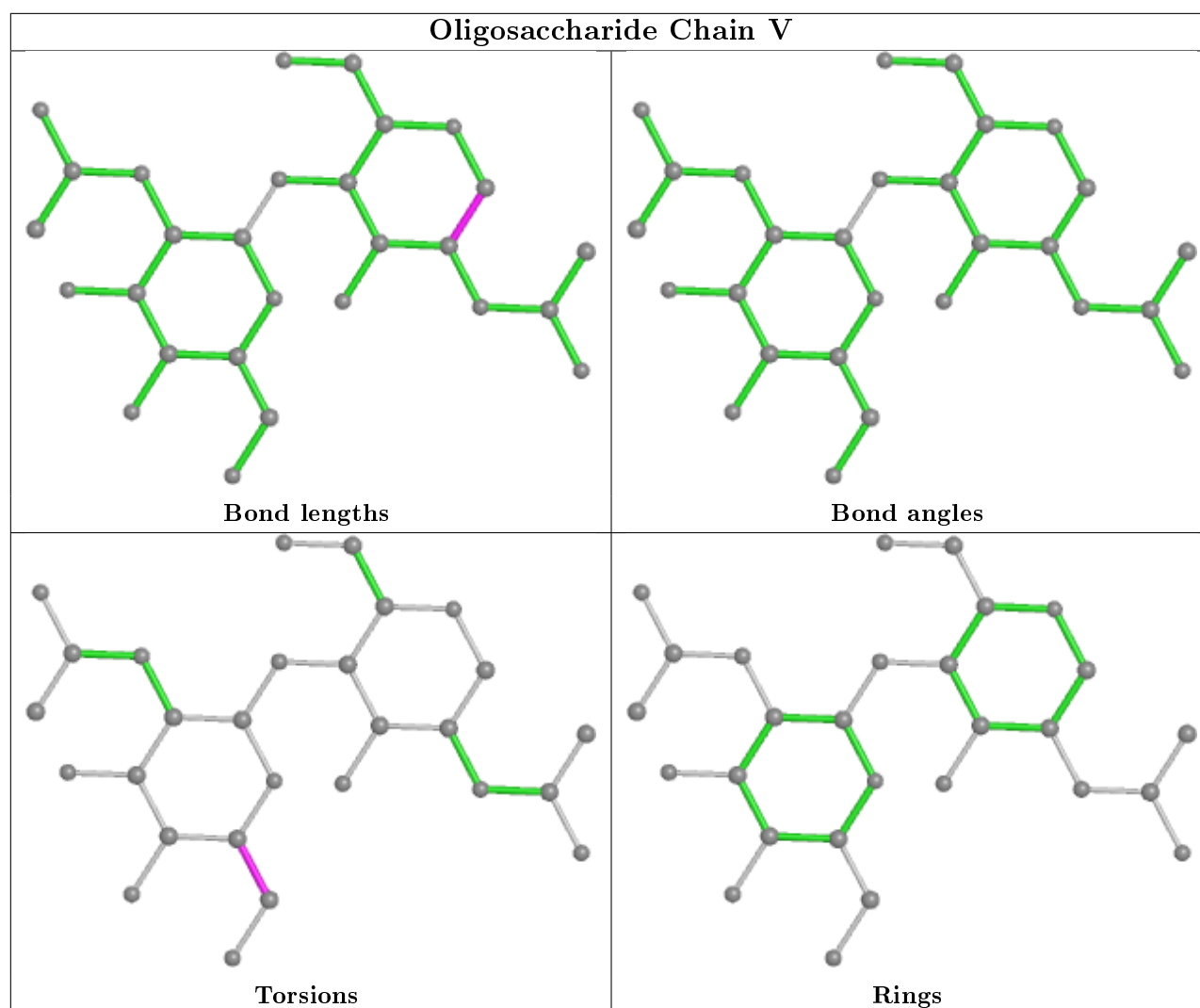


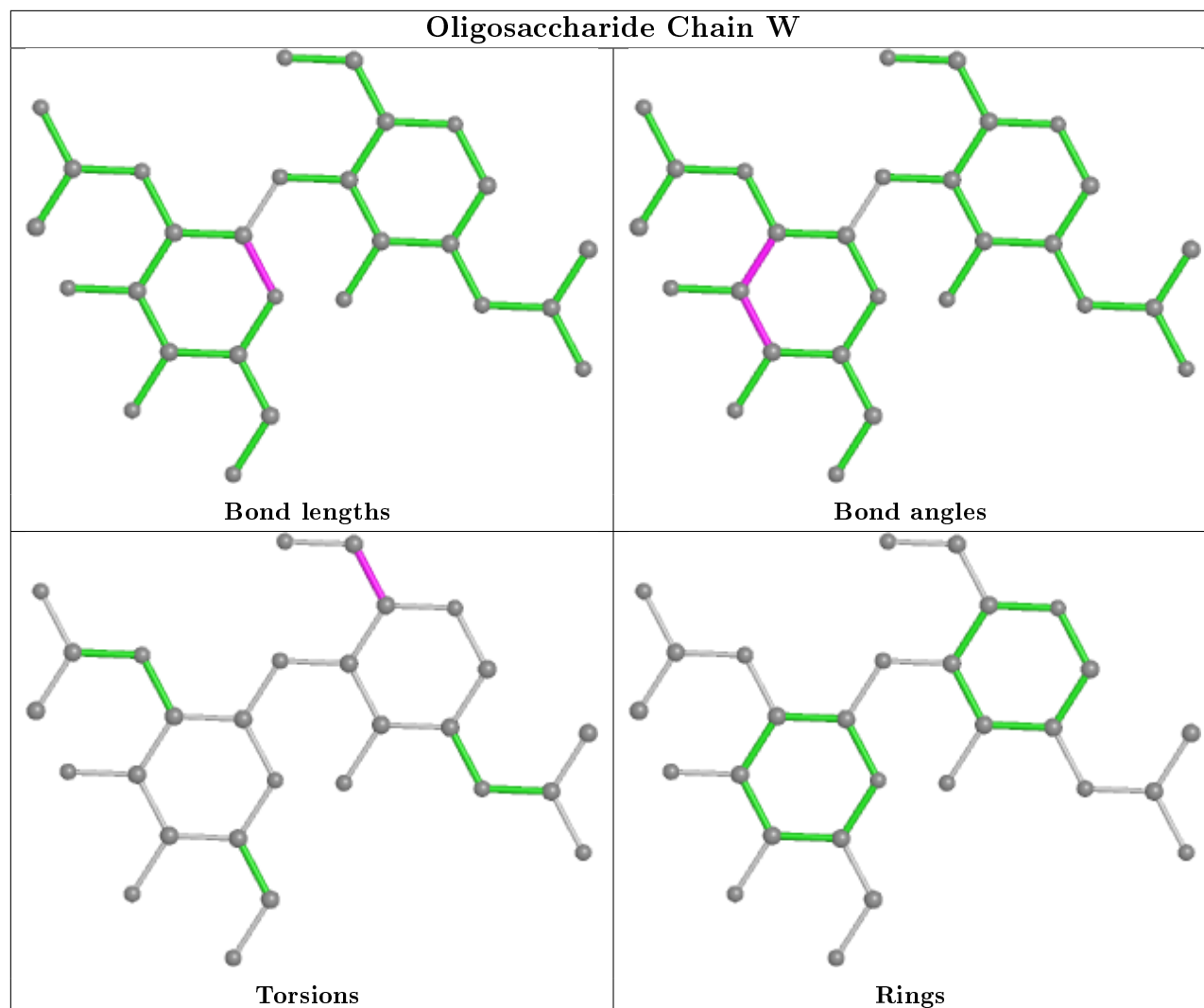


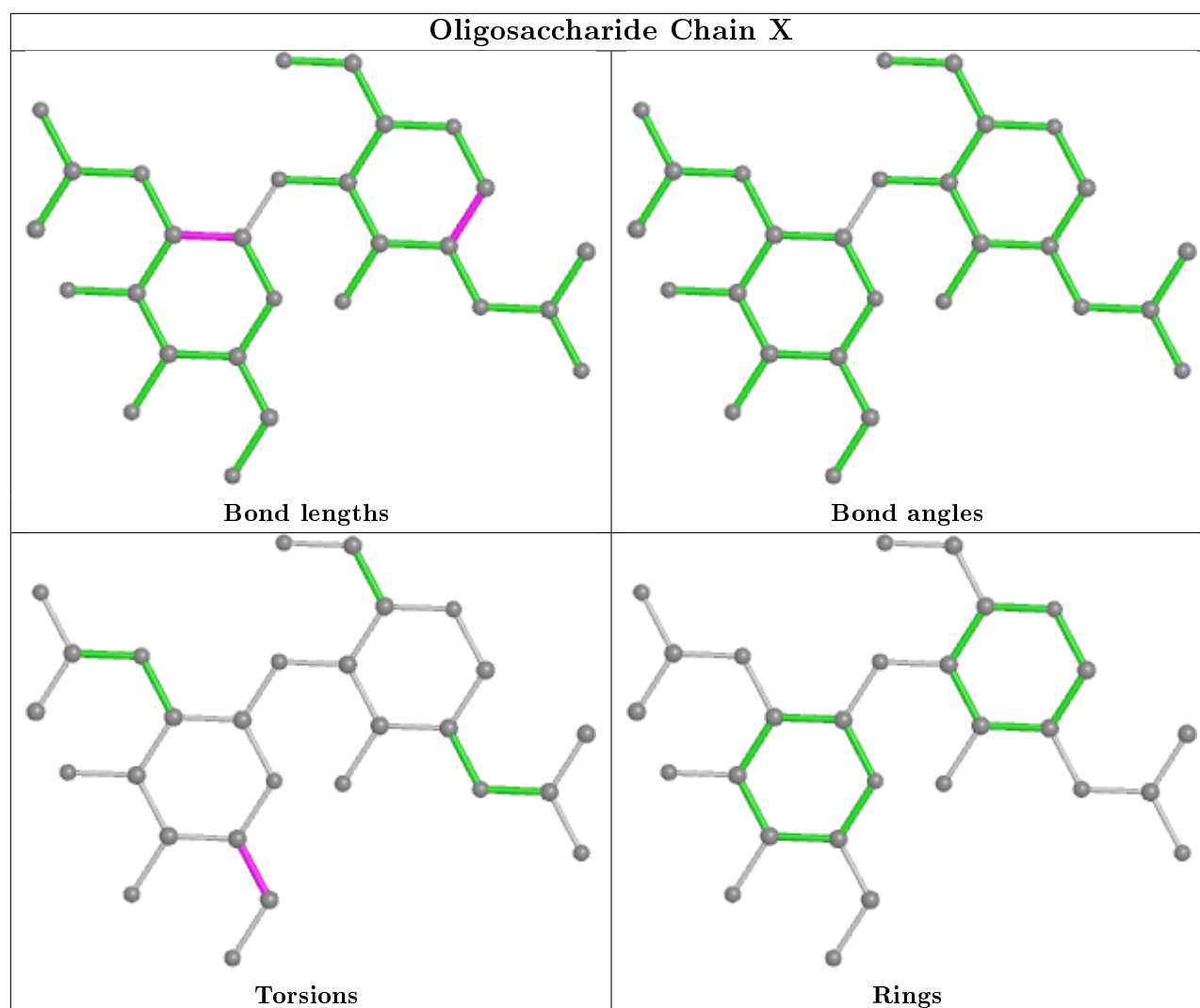












## 5.6 Ligand geometry ⓘ

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$
4	NAG	E	501	1	14,14,15	0.77	1 (7%)	17,19,21	1.17	2 (11%)
4	NAG	C	501	1	14,14,15	0.81	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	A	501	1	14,14,15	0.82	1 (7%)	17,19,21	1.21	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	K	501	1	14,14,15	0.85	1 (7%)	17,19,21	1.37	2 (11%)
4	NAG	I	501	1	14,14,15	0.82	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	G	501	1	14,14,15	0.76	1 (7%)	17,19,21	0.79	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
4	NAG	E	501	1	-	3/6/23/26	0/1/1/1
4	NAG	C	501	1	-	2/6/23/26	0/1/1/1
4	NAG	A	501	1	-	1/6/23/26	0/1/1/1
4	NAG	K	501	1	-	3/6/23/26	0/1/1/1
4	NAG	I	501	1	-	2/6/23/26	0/1/1/1
4	NAG	G	501	1	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	NAG	C1-C2	2.78	1.56	1.52
4	K	501	NAG	C1-C2	2.71	1.56	1.52
4	E	501	NAG	C1-C2	2.48	1.56	1.52
4	I	501	NAG	C1-C2	2.44	1.56	1.52
4	C	501	NAG	C1-C2	2.40	1.55	1.52
4	G	501	NAG	C1-C2	2.21	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	501	NAG	C2-N2-C7	3.67	128.13	122.90
4	K	501	NAG	C1-O5-C5	3.40	116.80	112.19
4	A	501	NAG	C2-N2-C7	3.19	127.45	122.90
4	E	501	NAG	C1-O5-C5	3.07	116.35	112.19
4	A	501	NAG	C1-O5-C5	2.81	116.00	112.19
4	C	501	NAG	C1-O5-C5	2.74	115.91	112.19
4	I	501	NAG	C1-O5-C5	2.74	115.90	112.19
4	E	501	NAG	C2-N2-C7	2.72	126.78	122.90
4	G	501	NAG	C1-O5-C5	2.29	115.30	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	501	NAG	O5-C5-C6-O6
4	I	501	NAG	O5-C5-C6-O6
4	G	501	NAG	C4-C5-C6-O6
4	I	501	NAG	C4-C5-C6-O6
4	C	501	NAG	O5-C5-C6-O6
4	K	501	NAG	C1-C2-N2-C7
4	C	501	NAG	C4-C5-C6-O6
4	A	501	NAG	C1-C2-N2-C7
4	E	501	NAG	C1-C2-N2-C7
4	K	501	NAG	C4-C5-C6-O6
4	E	501	NAG	C3-C2-N2-C7
4	E	501	NAG	O5-C5-C6-O6
4	K	501	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	501	NAG	1	0
4	A	501	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	319/335 (95%)	0.40	37 (11%) 4 1	12, 99, 167, 193	0
1	C	319/335 (95%)	-0.44	1 (0%) 94 84	9, 39, 80, 132	0
1	E	319/335 (95%)	0.39	40 (12%) 3 1	11, 99, 160, 206	0
1	G	319/335 (95%)	-0.40	0 100 100	12, 39, 81, 110	0
1	I	319/335 (95%)	-0.43	0 100 100	11, 40, 79, 116	0
1	K	319/335 (95%)	0.46	41 (12%) 3 1	12, 102, 164, 191	0
2	B	168/188 (89%)	-0.31	4 (2%) 59 30	10, 31, 124, 162	0
2	D	168/188 (89%)	-0.43	0 100 100	8, 26, 84, 150	0
2	F	168/188 (89%)	-0.38	4 (2%) 59 30	10, 31, 110, 162	0
2	H	168/188 (89%)	-0.43	1 (0%) 89 72	13, 25, 80, 147	0
2	J	168/188 (89%)	-0.44	0 100 100	11, 25, 81, 152	0
2	L	168/188 (89%)	-0.33	4 (2%) 59 30	9, 32, 112, 172	0
All	All	2922/3138 (93%)	-0.14	132 (4%) 33 12	8, 43, 148, 206	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	PHE	12.5
1	E	246	PHE	9.1
1	K	246	PHE	7.9
1	A	137	SER	7.7
1	E	127	TRP	7.0
1	K	202	ARG	7.0
1	A	127	TRP	6.9
2	B	60	ASN	6.6
1	E	226	ASN	6.5
2	L	60	ASN	6.2
1	A	151	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	K	138	ALA	5.8
1	K	127	TRP	5.7
1	A	167	VAL	5.4
1	K	165	ILE	5.1
1	A	226	ASN	5.0
1	E	253	ILE	4.8
1	E	223	ARG	4.8
1	A	205	VAL	4.7
1	A	253	ILE	4.7
1	E	202	ARG	4.7
1	A	252	LEU	4.7
1	E	167	VAL	4.6
1	A	215	VAL	4.6
2	B	63	TYR	4.5
2	B	62	LYS	4.4
1	E	168	THR	4.4
1	K	253	ILE	4.4
2	L	62	LYS	4.3
1	K	226	ASN	4.3
1	E	244	ILE	4.3
1	K	137	SER	4.2
1	A	202	ARG	4.2
1	E	218	ILE	4.1
1	E	224	VAL	4.0
1	K	245	ILE	4.0
1	K	168	THR	4.0
1	E	205	VAL	3.9
2	L	63	TYR	3.8
1	K	247	ASN	3.8
1	A	247	ASN	3.7
2	F	63	TYR	3.7
1	A	245	ILE	3.7
1	K	140	LEU	3.7
1	K	184	HIS	3.7
1	K	154	LEU	3.7
1	K	224	VAL	3.7
1	A	165	ILE	3.7
1	E	225	ARG	3.6
1	K	188	SER	3.6
1	E	138	ALA	3.4
1	E	165	ILE	3.4
1	K	205	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	180	LEU	3.4
1	E	137	SER	3.4
1	E	247	ASN	3.3
1	K	223	ARG	3.3
1	K	248	SER	3.3
1	K	233	ILE	3.2
1	E	220	SER	3.2
1	K	200	THR	3.1
2	F	62	LYS	3.1
1	E	229	GLY	3.1
1	E	186	PRO	3.0
1	K	244	ILE	3.0
2	F	60	ASN	3.0
1	E	184	HIS	2.9
1	A	244	ILE	2.9
1	E	252	LEU	2.9
1	E	201	GLY	2.9
1	A	227	GLN	2.8
1	K	56	LEU	2.8
1	A	225	ARG	2.8
1	K	252	LEU	2.8
1	K	218	ILE	2.8
2	L	61	GLU	2.8
1	K	125	PHE	2.8
1	A	136	SER	2.7
1	A	223	ARG	2.7
1	K	153	TRP	2.7
1	A	216	PRO	2.7
1	K	249	ILE	2.7
1	A	126	THR	2.7
1	A	164	PRO	2.7
1	K	291	GLN	2.7
2	B	61	GLU	2.7
1	E	215	VAL	2.6
1	A	213	SER	2.6
1	E	206	SER	2.6
1	A	218	ILE	2.5
1	A	224	VAL	2.5
1	K	221	ARG	2.5
1	K	151	LEU	2.5
1	A	125	PHE	2.5
1	E	183	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	186	PRO	2.5
1	E	212	ILE	2.5
1	C	158	THR	2.4
1	E	245	ILE	2.4
1	K	230	ARG	2.4
1	A	184	HIS	2.4
1	K	229	GLY	2.4
1	E	204	THR	2.4
2	F	56	ILE	2.4
1	A	56	LEU	2.4
1	A	275	ARG	2.4
1	K	215	VAL	2.4
1	A	168	THR	2.3
1	E	211	GLN	2.3
1	K	183	VAL	2.3
1	A	66	LEU	2.3
1	E	154	LEU	2.3
1	E	182	GLY	2.3
1	E	98	TYR	2.3
1	K	167	VAL	2.3
1	A	203	VAL	2.2
1	A	154	LEU	2.2
1	E	227	GLN	2.2
1	K	216	PRO	2.2
1	K	220	SER	2.2
1	E	124	GLN	2.2
1	A	124	GLN	2.1
1	E	213	SER	2.1
1	E	230	ARG	2.1
1	E	140	LEU	2.1
1	K	206	SER	2.1
1	K	126	THR	2.0
1	E	216	PRO	2.0
2	H	58	LYS	2.0
1	A	221	ARG	2.0
1	E	56	LEU	2.0
1	A	162	TYR	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 ⓘ

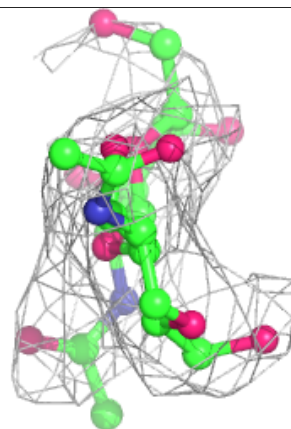
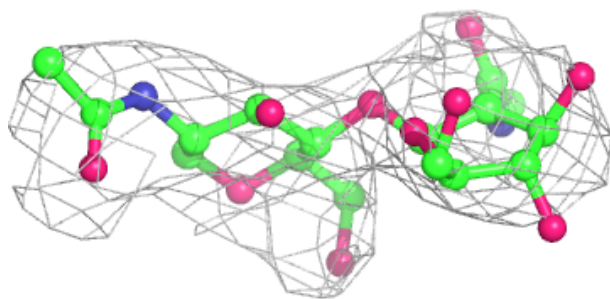
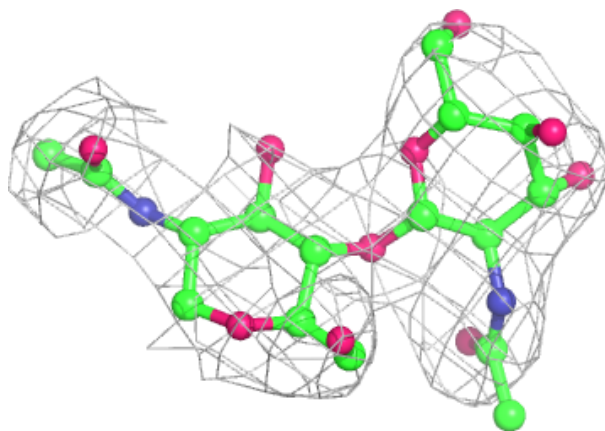
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	R	2	14/15	0.82	0.28	54,67,78,80	0
3	NAG	X	2	14/15	0.82	0.23	46,61,76,78	0
3	NAG	P	2	14/15	0.86	0.15	34,58,72,73	0
3	NAG	N	2	14/15	0.87	0.29	57,67,74,75	0
3	NAG	O	2	14/15	0.87	0.17	69,79,85,94	0
3	NAG	Q	2	14/15	0.88	0.22	78,103,113,117	0
3	NAG	V	2	14/15	0.88	0.15	48,66,82,82	0
3	NAG	M	2	14/15	0.89	0.20	79,95,101,102	0
3	NAG	N	1	14/15	0.89	0.17	55,66,70,73	0
3	NAG	T	2	14/15	0.89	0.14	43,64,68,70	0
3	NAG	U	2	14/15	0.90	0.15	67,70,74,78	0
3	NAG	W	2	14/15	0.90	0.16	69,91,97,101	0
3	NAG	M	1	14/15	0.91	0.18	54,63,75,86	0
3	NAG	P	1	14/15	0.91	0.14	53,66,70,73	0
3	NAG	V	1	14/15	0.91	0.14	44,64,74,78	0
3	NAG	R	1	14/15	0.91	0.14	50,60,73,75	0
3	NAG	X	1	14/15	0.92	0.14	55,63,69,73	0
3	NAG	T	1	14/15	0.93	0.15	43,55,67,68	0
3	NAG	S	2	14/15	0.93	0.15	49,75,79,80	0
3	NAG	W	1	14/15	0.94	0.14	60,67,79,91	0
3	NAG	Q	1	14/15	0.94	0.15	48,72,81,91	0
3	NAG	S	1	14/15	0.95	0.13	31,39,50,62	0
3	NAG	O	1	14/15	0.97	0.12	24,33,43,64	0
3	NAG	U	1	14/15	0.97	0.12	21,32,43,58	0

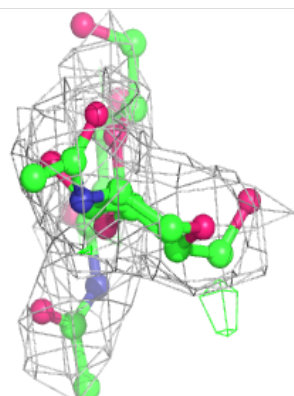
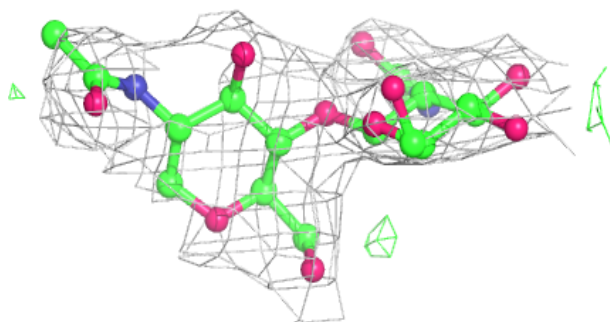
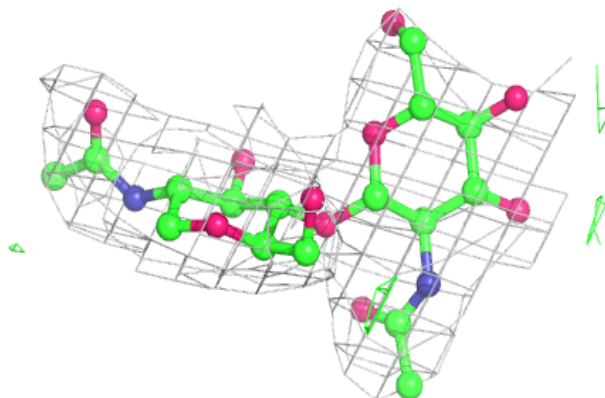
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain M:**

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

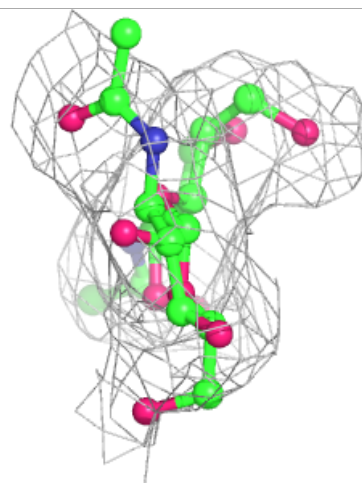
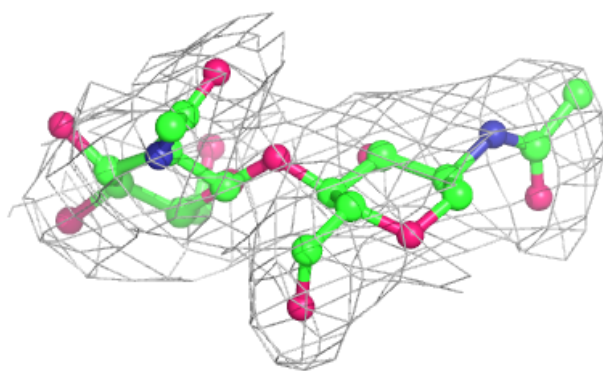
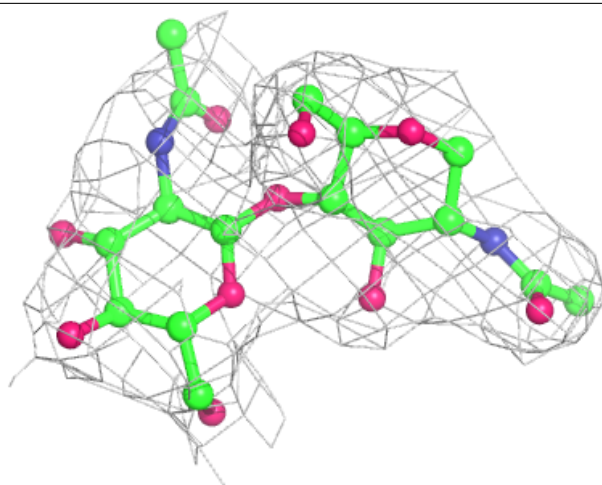
**Electron density around Chain N:**

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



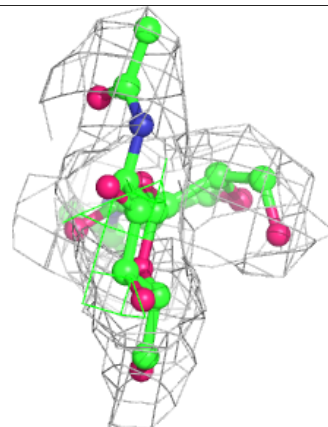
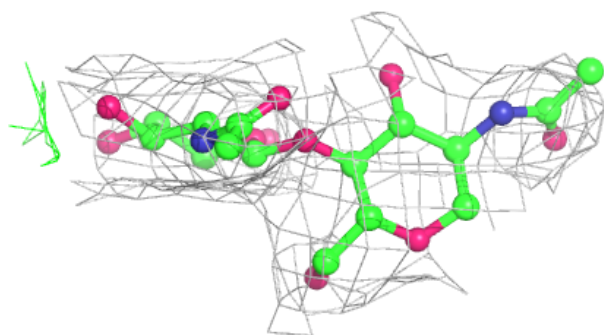
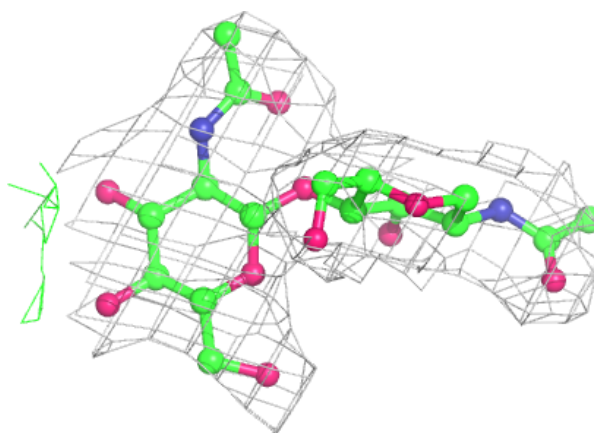
**Electron density around Chain O:**

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



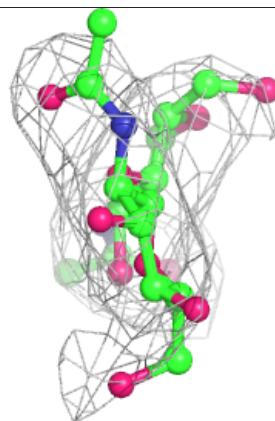
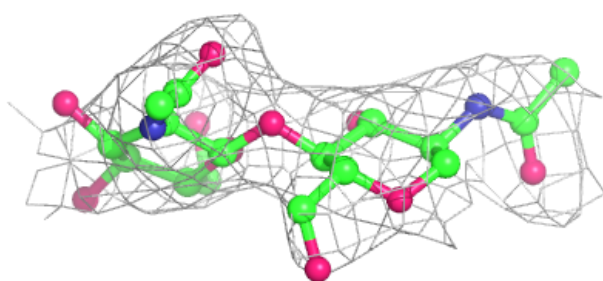
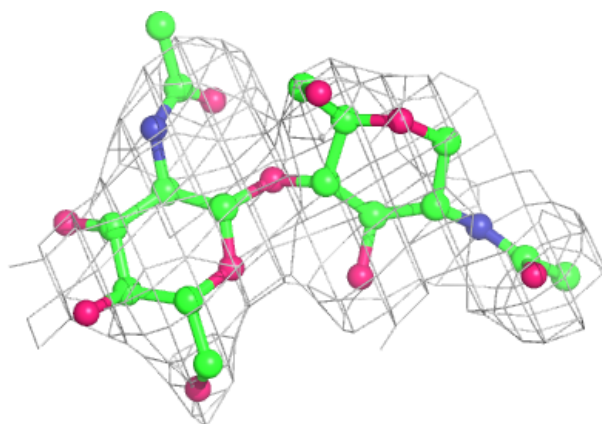
**Electron density around Chain P:**

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

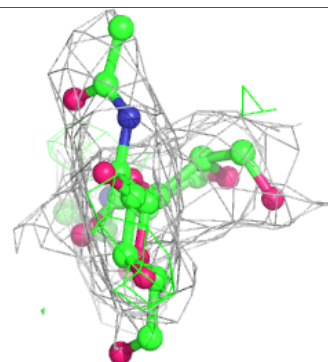
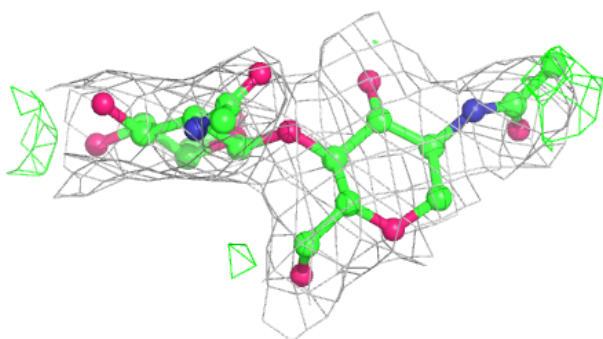
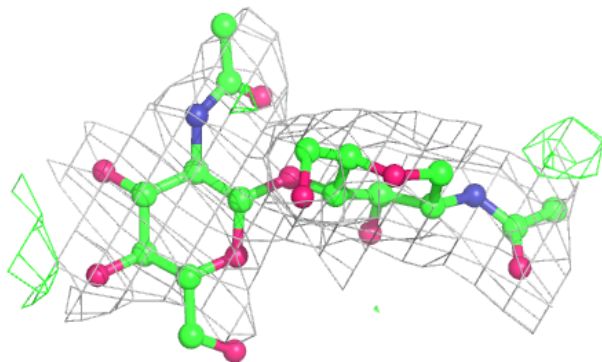


**Electron density around Chain Q:**

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

**Electron density around Chain R:**

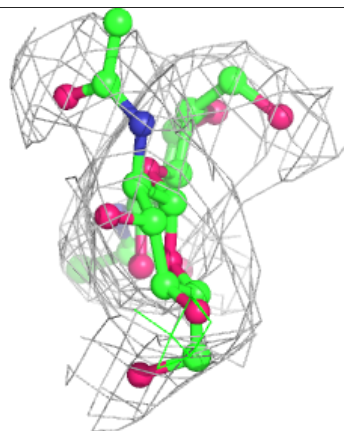
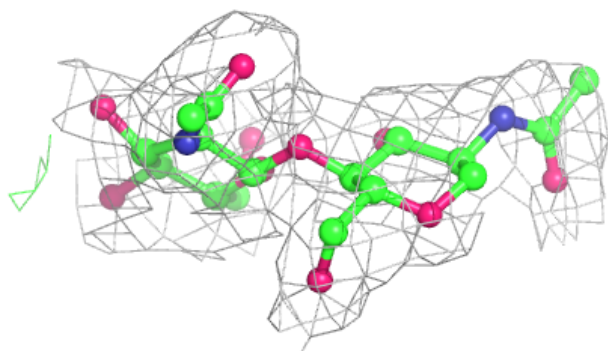
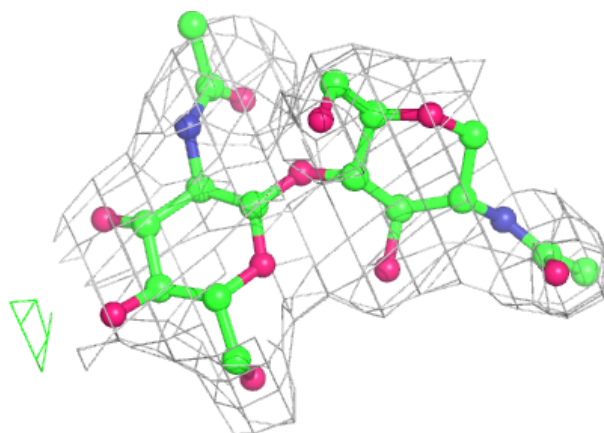
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





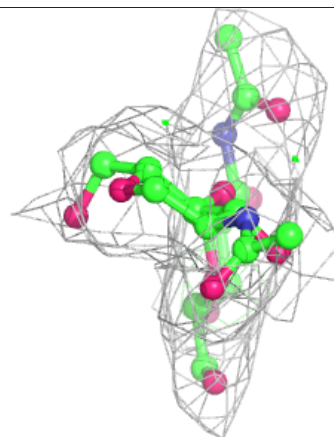
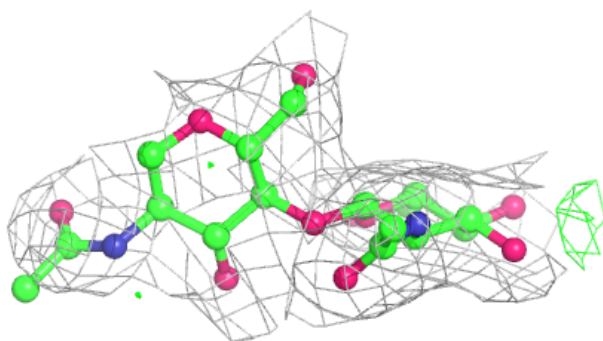
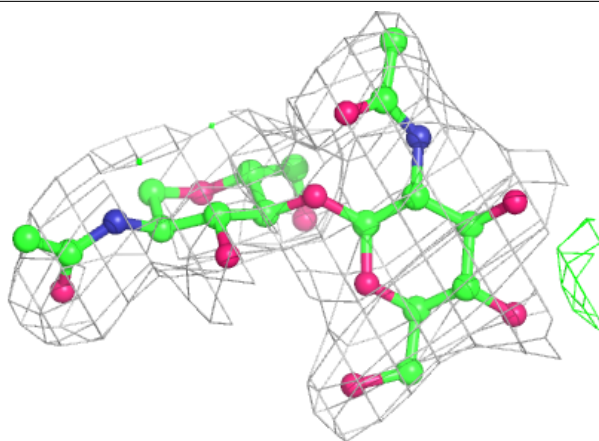
**Electron density around Chain S:**

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



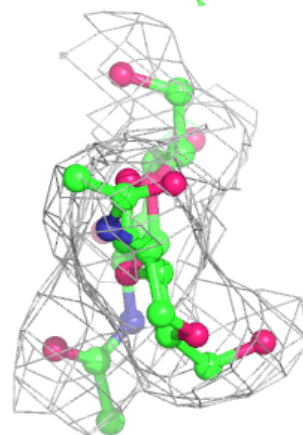
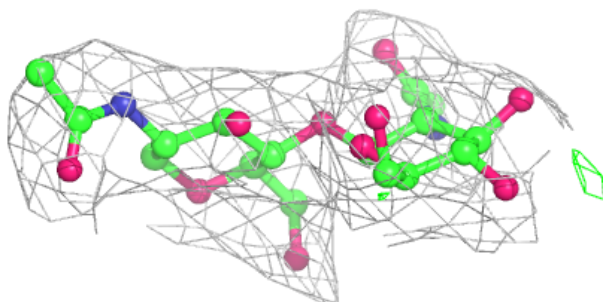
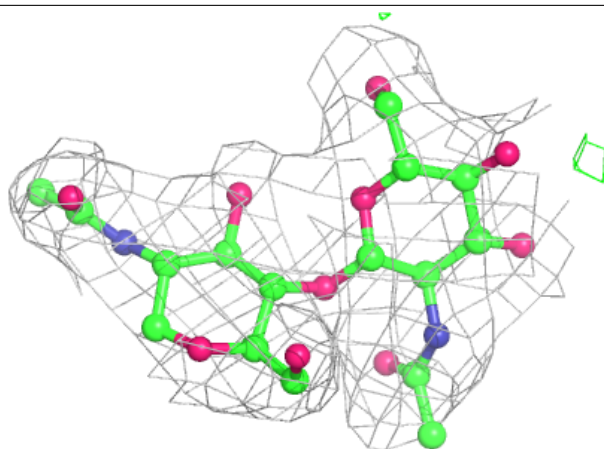
**Electron density around Chain T:**

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

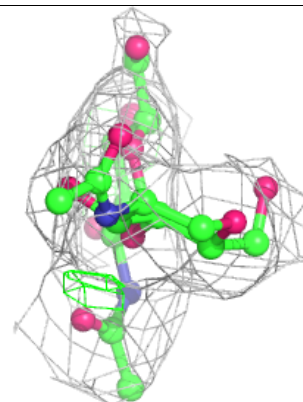
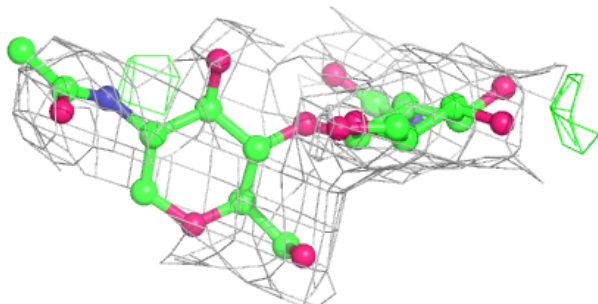
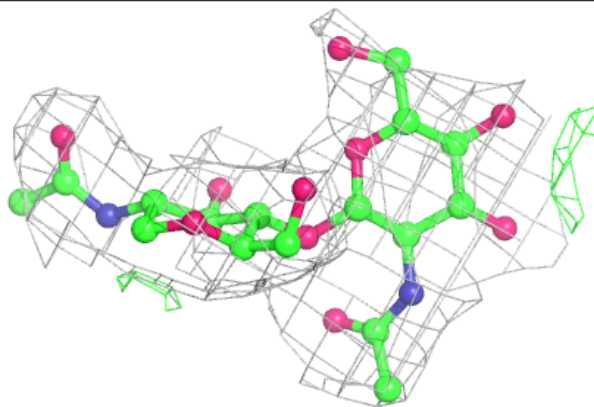


**Electron density around Chain U:**

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

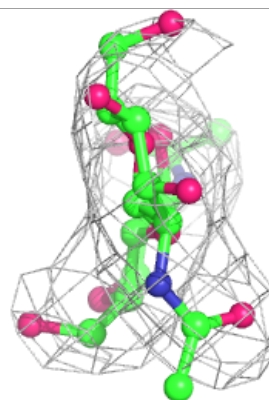
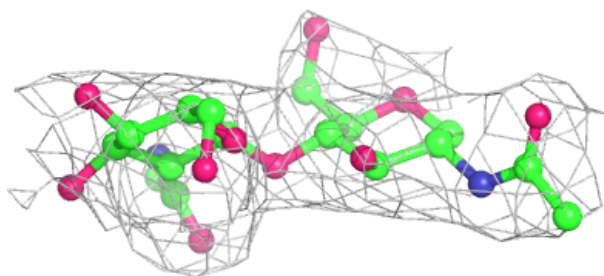
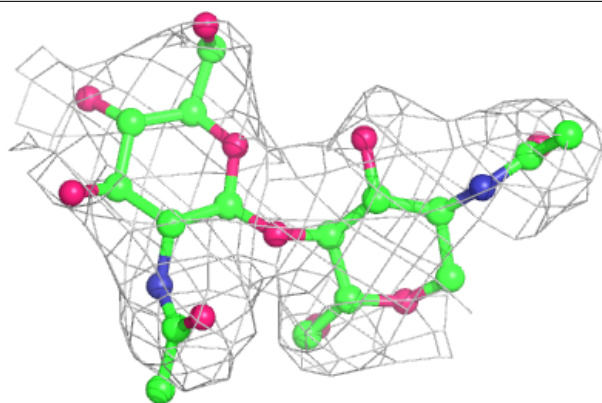
**Electron density around Chain V:**

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

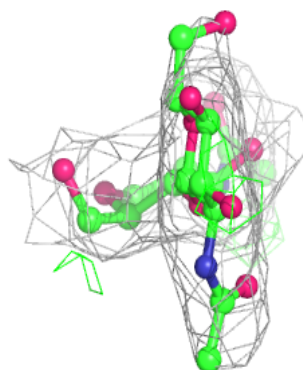
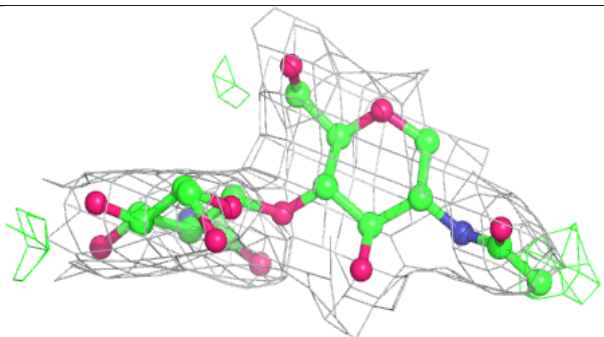
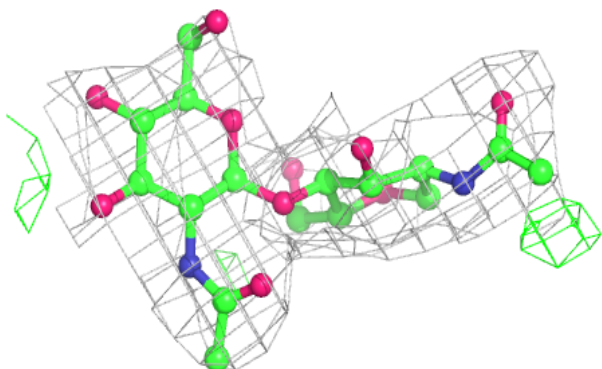


**Electron density around Chain W:**

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

**Electron density around Chain X:**

$2mF_o-DF_c$  (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
4	NAG	K	501	14/15	0.81	0.50	175,177,181,184	0
4	NAG	A	501	14/15	0.83	0.34	168,173,182,186	0
4	NAG	E	501	14/15	0.83	0.41	165,177,180,183	0
4	NAG	C	501	14/15	0.84	0.25	82,101,108,109	0
4	NAG	G	501	14/15	0.85	0.25	87,99,104,105	0
4	NAG	I	501	14/15	0.86	0.19	74,94,100,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.