



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:38 AM BST

PDB ID : 5X4A  
Title : SLL-2-Forssman antigen tetrasaccharides complex  
Authors : Kita, A.; Miki, K.  
Deposited on : 2017-02-11  
Resolution : 3.40 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

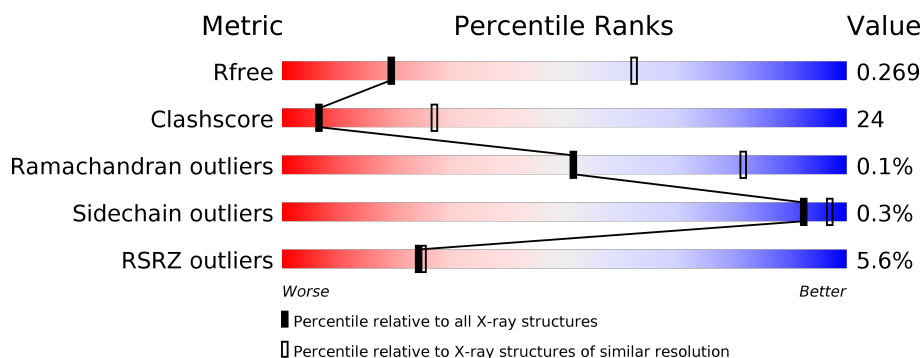
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	94	<div> <div></div> <div>63%37%</div> </div>
1	B	94	<div> <div></div> <div>60%39%</div> </div>
1	C	94	<div> <div></div> <div>60%40%</div> </div>
1	D	94	<div> <div></div> <div>54%46%</div> </div>
1	E	94	<div> <div>%</div> <div>64%36%</div> </div>
1	F	94	<div> <div>%</div> <div>63%37%</div> </div>




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Mol	Chain	Length	Quality of chain
1	G	94	<div> <div>2%</div> <div>55%</div> <div>45%</div> </div>
1	H	94	<div> <div>%</div> <div>56%</div> <div>41%</div> <div>.</div> </div>
1	I	94	<div> <div>59%</div> <div>41%</div> </div>
1	J	94	<div> <div>10%</div> <div>82%</div> <div>18%</div> </div>
1	K	94	<div> <div>18%</div> <div>69%</div> <div>30%</div> <div>.</div> </div>
1	L	94	<div> <div>34%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
2	M	2	<div> <div>50%</div> <div>50%</div> </div>
2	O	2	<div> <div>50%</div> <div>50%</div> </div>
2	Q	2	<div> <div>50%</div> <div>50%</div> </div>
2	R	2	<div> <div>50%</div> <div>50%</div> </div>
2	T	2	<div> <div>50%</div> <div>50%</div> </div>
2	V	2	<div> <div>50%</div> <div>50%</div> </div>
2	X	2	<div> <div>50%</div> <div>50%</div> </div>
2	Z	2	<div> <div>100%</div> </div>
2	b	2	<div> <div>100%</div> </div>
2	c	2	<div> <div>100%</div> </div>
2	e	2	<div> <div>100%</div> </div>
2	g	2	<div> <div>100%</div> </div>
3	N	4	<div> <div>100%</div> </div>
3	P	4	<div> <div>100%</div> </div>
3	S	4	<div> <div>75%</div> <div>25%</div> </div>
3	U	4	<div> <div>75%</div> <div>25%</div> </div>
3	W	4	<div> <div>100%</div> </div>
3	Y	4	<div> <div>50%</div> <div>50%</div> </div>
3	a	4	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	d	4	 100%
3	f	4	 100%
3	h	4	 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
2	NAG	Z	1	-	-	X	-
2	NAG	c	2	-	-	-	X
2	NAG	e	2	-	-	-	X
3	GAL	N	1	-	-	-	X
3	NGA	W	3	-	-	X	-
3	NGA	d	3	-	-	-	X
3	GAL	f	1	-	-	-	X
4	GLA	A	107	-	-	X	-

## 2 Entry composition

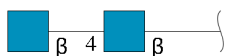
There are 5 unique types of molecules in this entry. The entry contains 9927 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Galactose-binding lectin.

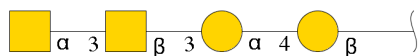
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			759	479	129	145	6			
1	B	94	Total	C	N	O	S	0	0	0
			755	477	129	143	6			
1	C	94	Total	C	N	O	S	0	0	0
			759	479	129	145	6			
1	D	94	Total	C	N	O	S	0	0	0
			755	477	129	143	6			
1	E	94	Total	C	N	O	S	0	0	0
			759	479	129	145	6			
1	F	94	Total	C	N	O	S	0	0	0
			759	479	129	145	6			
1	G	94	Total	C	N	O	S	0	0	0
			759	479	129	145	6			
1	H	94	Total	C	N	O	S	0	0	0
			759	479	129	145	6			
1	I	94	Total	C	N	O	S	0	0	0
			755	477	129	143	6			
1	J	94	Total	C	N	O	S	0	0	0
			752	473	129	144	6			
1	K	94	Total	C	N	O	S	0	0	0
			753	476	126	145	6			
1	L	94	Total	C	N	O	S	0	0	0
			744	472	122	144	6			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	e	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	g	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



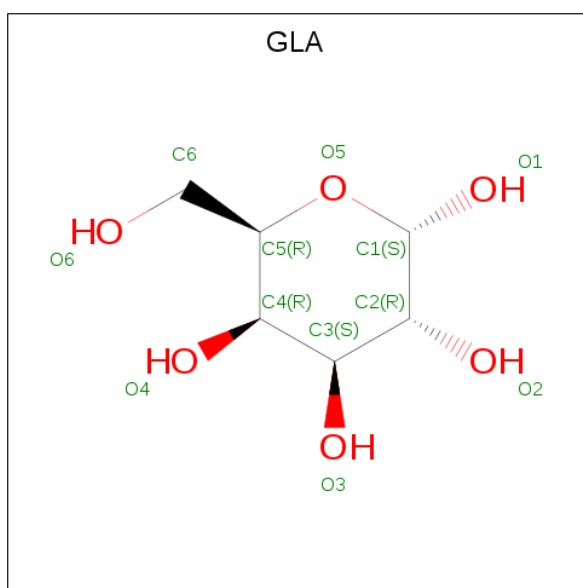
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	N	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	P	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	S	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	U	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	W	4	Total	C	N	O	0	0	0
			51	28	2	21			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Y	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	a	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	d	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	f	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	h	4	Total	C	N	O	0	0	0
			51	28	2	21			

- Molecule 4 is alpha-D-galactopyranose (three-letter code: GLA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	O	0	0
			1	1		

### 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: Galactose-binding lectin

Chain A: 



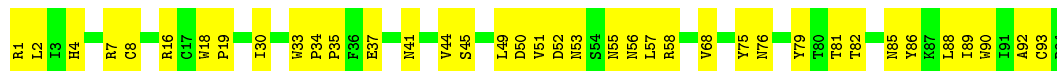
- Molecule 1: Galactose-binding lectin

Chain B: 



- Molecule 1: Galactose-binding lectin

Chain C: 



- Molecule 1: Galactose-binding lectin

Chain D: 



- Molecule 1: Galactose-binding lectin

Chain E: 



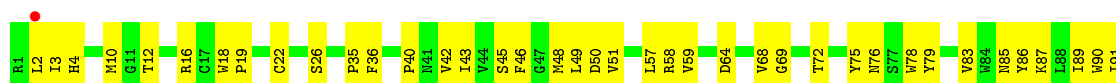
- Molecule 1: Galactose-binding lectin

Chain F: 





- Molecule 1: Galactose-binding lectin



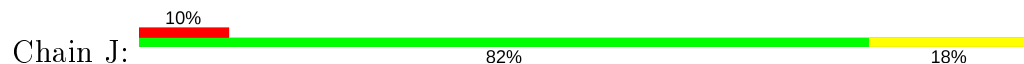
- Molecule 1: Galactose-binding lectin



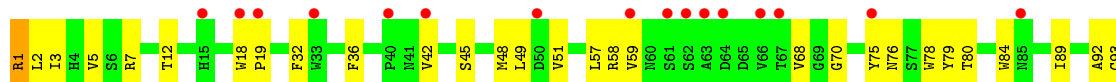
- Molecule 1: Galactose-binding lectin



- Molecule 1: Galactose-binding lectin

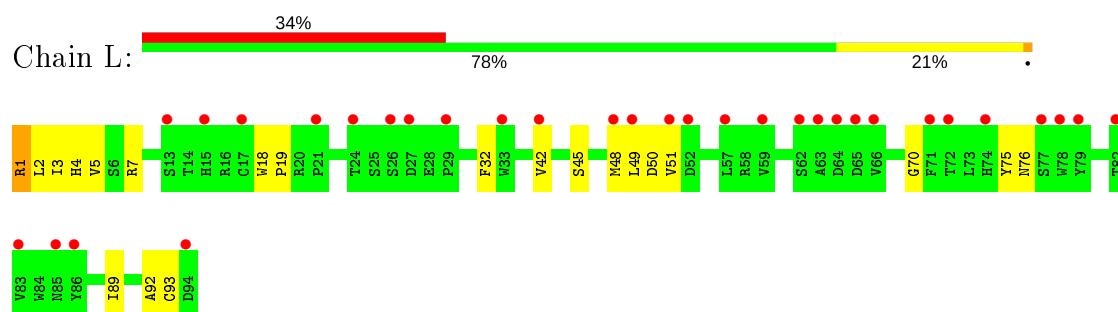


- Molecule 1: Galactose-binding lectin



- Molecule 1: Galactose-binding lectin





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



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



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



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



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



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

Chain V:  50% 50%

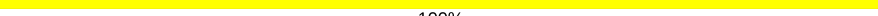
HA01  
HA02

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

Chain X:  50% 50%

HA01  
HA02

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

Chain Z:  100%

HA01  
HA02

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

Chain b:  100%

HA01  
HA02

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

Chain c:  100%


HA01  
HA02

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

Chain e:  100%

HA01  
HA02

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

Chain g:  100%

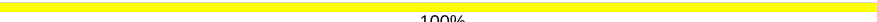
HA01  
HA02

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

Chain N:  100%

GAL1  
GLA2  
NGA3  
A2G4

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

Chain P:  100%

GAL1  
GLA2  
NGA3  
A2G4

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

Chain S:  75% 25%

GAL1  
GLA2  
NGA3  
A2G4

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

Chain U:  75% 25%

GAL1  
GLA2  
NGA3  
A2G4

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

Chain W:  100%

GAL1  
GLA2  
NGA3  
A2G4

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

Chain Y:  50% 50%

GAL1  
GLA2  
NGA3  
A2G4

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

Chain a:  100%

GM1  
GLA2  
NGA3  
A2G4

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

Chain d:  100%

GM1  
GLA2  
NGA3  
A2G4

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

Chain f:  100%

GM1  
GLA2  
NGA3  
A2G4

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

Chain h:  100%

GM1  
GLA2  
NGA3  
A2G4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.47Å 99.94Å 273.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.40 48.75 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.6 (100.00-3.40) 96.8 (48.75-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.99 (at 3.40Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.239 , 0.266 0.237 , 0.269	Depositor DCC
$R_{free}$ test set	1794 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 66.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9927	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	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 21.38 % 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  $7.0965e-03$ . 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, GAL, NAG, NGA, A2G

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	0.80	0/784	0.85	0/1075
1	B	0.71	0/780	0.85	1/1070 (0.1%)
1	C	0.75	0/784	0.84	1/1075 (0.1%)
1	D	0.69	0/780	0.86	0/1070
1	E	0.68	0/784	0.83	0/1075
1	F	0.64	0/784	0.82	0/1075
1	G	0.61	0/784	0.75	0/1075
1	H	0.67	0/784	0.79	1/1075 (0.1%)
1	I	0.62	0/780	0.72	0/1070
1	J	0.72	0/776	0.74	0/1064
1	K	0.82	0/778	0.77	1/1068 (0.1%)
1	L	0.81	0/769	0.78	0/1057
All	All	0.71	0/9367	0.80	4/12849 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	K	48	MET	CG-SD-CE	5.32	108.70	100.20
1	C	41	ASN	N-CA-C	-5.10	97.22	111.00
1	B	10	MET	CG-SD-CE	5.01	108.21	100.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	759	0	700	55	0
1	B	755	0	696	55	0
1	C	759	0	700	42	0
1	D	755	0	696	48	0
1	E	759	0	700	45	0
1	F	759	0	700	53	0
1	G	759	0	700	41	0
1	H	759	0	700	48	0
1	I	755	0	696	48	0
1	J	752	0	693	19	0
1	K	753	0	689	28	0
1	L	744	0	674	23	0
2	M	28	0	25	1	0
2	O	28	0	25	1	0
2	Q	28	0	25	1	0
2	R	28	0	25	6	0
2	T	28	0	25	4	0
2	V	28	0	25	3	0
2	X	28	0	25	5	0
2	Z	28	0	25	8	0
2	b	28	0	25	0	0
2	c	28	0	25	0	0
2	e	28	0	25	0	0
2	g	28	0	25	0	0
3	N	51	0	44	3	0
3	P	51	0	44	4	0
3	S	51	0	44	3	0
3	U	51	0	44	3	0
3	W	51	0	44	9	0
3	Y	51	0	44	5	0
3	a	51	0	44	0	0
3	d	51	0	44	0	0
3	f	51	0	44	0	0
3	h	51	0	44	0	0
4	A	12	0	12	12	0
5	I	1	0	0	0	0
All	All	9927	0	9096	421	0



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (421) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:HIS:CE1	1:E:2:LEU:HD21	1.24	1.64
1:H:16:ARG:HH22	2:X:1:NAG:C8	1.31	1.43
1:H:16:ARG:NH2	2:X:1:NAG:H83	1.09	1.38
1:B:4:HIS:CE1	1:E:2:LEU:CD2	2.06	1.34
1:A:2:LEU:HD21	1:F:4:HIS:CE1	1.75	1.21
1:E:16:ARG:NH2	2:R:1:NAG:H83	1.57	1.19
1:I:16:ARG:HH12	2:Z:1:NAG:H83	1.02	1.17
1:H:16:ARG:NH2	2:X:1:NAG:C8	1.98	1.16
1:D:16:ARG:NH2	2:V:1:NAG:H83	1.61	1.15
1:F:16:ARG:HH21	2:T:1:NAG:H83	1.15	1.08
1:H:42:VAL:HG22	1:H:92:ALA:HB2	1.34	1.04
1:D:16:ARG:HH22	2:V:1:NAG:H83	0.87	1.01
1:A:2:LEU:CD2	1:F:4:HIS:CE1	2.45	1.00
1:I:16:ARG:NH1	2:Z:1:NAG:H83	1.77	0.98
1:L:18:TRP:CD1	1:L:19:PRO:HA	1.99	0.97
1:F:16:ARG:NH2	2:T:1:NAG:H83	1.83	0.93
1:B:2:LEU:HD21	1:E:4:HIS:CE1	2.05	0.91
1:B:4:HIS:ND1	1:E:2:LEU:CD2	2.35	0.89
1:E:16:ARG:NH2	2:R:1:NAG:C8	2.37	0.87
1:A:84:TRP:NE1	4:A:107:GLA:H61	1.90	0.86
1:I:32:PHE:C	1:I:33:TRP:HD1	1.78	0.85
1:D:42:VAL:HG22	1:D:92:ALA:HB2	1.57	0.84
1:I:32:PHE:O	1:I:33:TRP:HD1	1.60	0.84
1:B:4:HIS:HE1	1:E:2:LEU:HD21	1.04	0.84
1:C:18:TRP:CD1	1:C:19:PRO:HA	2.12	0.83
1:A:84:TRP:CD1	4:A:107:GLA:H61	2.12	0.83
1:A:84:TRP:CD1	4:A:107:GLA:O6	2.32	0.83
1:B:16:ARG:NH2	2:M:1:NAG:H83	1.96	0.81
1:A:84:TRP:CD1	4:A:107:GLA:C6	2.64	0.81
1:H:42:VAL:HG22	1:H:92:ALA:CB	2.11	0.80
1:C:50:ASP:HB3	1:C:85:ASN:H	1.47	0.80
1:H:39:THR:HG23	1:H:66:VAL:HG12	1.64	0.80
1:G:26:SER:OG	1:G:75:TYR:HB3	1.83	0.79
1:I:16:ARG:HH12	2:Z:1:NAG:C8	1.91	0.78
1:G:12:THR:HG22	1:G:89:ILE:HG22	1.66	0.77
1:F:79:TYR:CZ	3:W:3:NGA:H4	2.20	0.76
1:B:4:HIS:ND1	1:E:2:LEU:HD21	1.93	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:VAL:HG22	1:F:83:VAL:HG22	1.67	0.76
1:F:42:VAL:HG22	1:F:92:ALA:HB2	1.67	0.75
1:G:89:ILE:HD11	1:I:45:SER:HB2	1.67	0.75
1:B:4:HIS:ND1	1:E:2:LEU:HD23	2.03	0.74
1:I:32:PHE:C	1:I:33:TRP:CD1	2.62	0.74
1:D:33:TRP:CE3	1:D:34:PRO:HA	2.22	0.73
1:D:1:ARG:HH11	1:D:1:ARG:HG2	1.51	0.73
1:A:56:ASN:OD1	1:B:52:ASP:HA	1.89	0.73
1:E:16:ARG:HH21	2:R:1:NAG:H83	1.54	0.73
1:G:4:HIS:CE1	1:L:2:LEU:HD21	2.24	0.73
1:B:20:ARG:HD2	1:B:21:PRO:O	1.88	0.72
1:A:19:PRO:O	1:A:84:TRP:HZ3	1.73	0.72
1:G:2:LEU:HG	1:L:4:HIS:CE1	2.24	0.72
1:B:79:TYR:CD2	1:B:80:THR:HG23	2.25	0.71
1:I:16:ARG:HH22	2:Z:1:NAG:HN2	1.38	0.71
1:D:89:ILE:HD12	1:F:43:ILE:HD12	1.72	0.71
1:H:18:TRP:CD1	1:H:19:PRO:HA	2.26	0.70
1:A:79:TYR:HB2	3:N:4:A2G:O7	1.92	0.70
1:F:36:PHE:HD2	1:F:94:ASP:OD2	1.74	0.70
1:I:7:ARG:O	1:I:93:CYS:HA	1.91	0.70
1:F:81:THR:HG22	1:F:82:THR:N	2.07	0.70
1:A:48:MET:O	1:A:86:TYR:HA	1.92	0.70
1:F:58:ARG:HD2	1:F:78:TRP:O	1.93	0.69
1:A:84:TRP:CE2	4:A:107:GLA:H61	2.27	0.69
1:H:1:ARG:N	1:K:5:VAL:O	2.22	0.69
1:E:42:VAL:HG22	1:E:92:ALA:HB2	1.75	0.68
1:H:39:THR:CG2	1:H:66:VAL:HG12	2.24	0.68
1:D:44:VAL:HG22	1:D:90:TRP:HB3	1.73	0.68
1:A:45:SER:HB2	1:B:89:ILE:CD1	2.23	0.68
1:A:84:TRP:NE1	4:A:107:GLA:C6	2.56	0.68
1:E:42:VAL:HG22	1:E:92:ALA:CB	2.24	0.68
1:H:2:LEU:HD22	1:K:2:LEU:HD22	1.77	0.67
1:E:16:ARG:HH22	2:R:1:NAG:H83	1.59	0.67
1:A:52:ASP:HB2	1:A:84:TRP:HE1	1.59	0.67
1:C:4:HIS:CE1	1:D:2:LEU:HG	2.30	0.67
1:F:58:ARG:HB3	1:F:78:TRP:CD2	2.30	0.67
1:D:7:ARG:O	1:D:93:CYS:HA	1.95	0.67
1:C:44:VAL:HG12	1:C:45:SER:N	2.10	0.67
4:A:107:GLA:O2	1:C:79:TYR:CD2	2.44	0.67
1:B:2:LEU:CD2	1:E:4:HIS:CE1	2.77	0.66
1:I:2:LEU:HD22	1:J:2:LEU:HD22	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:107:GLA:O6	1:C:56:ASN:ND2	2.30	0.65
1:B:4:HIS:CE1	1:E:2:LEU:HD23	2.23	0.65
1:B:45:SER:HB2	1:C:89:ILE:HD11	1.77	0.65
1:B:45:SER:HB2	1:C:89:ILE:CD1	2.27	0.65
1:H:45:SER:HB2	1:I:89:ILE:HD11	1.79	0.64
1:G:57:LEU:O	1:H:50:ASP:HA	1.97	0.64
1:B:1:ARG:HG2	1:B:1:ARG:HH11	1.61	0.64
1:D:7:ARG:HD2	1:F:4:HIS:CB	2.28	0.64
1:H:45:SER:HB2	1:I:89:ILE:CD1	2.28	0.64
1:B:18:TRP:CG	1:B:19:PRO:HA	2.33	0.64
4:A:107:GLA:O2	1:C:79:TYR:CE2	2.52	0.63
1:G:75:TYR:CG	1:G:76:ASN:N	2.67	0.63
1:G:42:VAL:HG22	1:G:92:ALA:CB	2.29	0.62
1:G:89:ILE:CD1	1:I:45:SER:HB2	2.28	0.62
1:D:17:CYS:O	1:D:20:ARG:N	2.31	0.62
1:A:45:SER:HB2	1:B:89:ILE:HD13	1.81	0.62
1:G:79:TYR:HB2	3:Y:4:A2G:O7	1.99	0.62
1:D:16:ARG:NH2	2:V:1:NAG:C8	2.51	0.61
1:H:16:ARG:CZ	2:X:1:NAG:H83	2.15	0.61
1:F:7:ARG:HB3	1:F:94:ASP:OD1	2.00	0.61
1:J:75:TYR:C	1:J:75:TYR:CD2	2.71	0.61
1:C:75:TYR:HB2	1:C:88:LEU:HD11	1.82	0.61
1:F:58:ARG:HD3	1:F:78:TRP:CD1	2.36	0.61
1:F:16:ARG:HH21	2:T:1:NAG:C8	2.03	0.61
1:K:45:SER:HB2	1:L:89:ILE:CD1	2.31	0.60
1:D:1:ARG:HG2	1:D:1:ARG:NH1	2.16	0.60
1:F:18:TRP:CD1	1:F:19:PRO:HA	2.36	0.60
1:E:16:ARG:HH22	2:R:1:NAG:C8	2.13	0.60
1:E:45:SER:HB2	1:F:89:ILE:HD11	1.82	0.60
1:B:1:ARG:HG2	1:B:1:ARG:NH1	2.15	0.59
1:K:18:TRP:CD1	1:K:19:PRO:HA	2.37	0.59
1:H:16:ARG:NH2	2:X:1:NAG:C7	2.64	0.59
1:D:45:SER:HB2	1:E:89:ILE:HD11	1.85	0.59
1:G:4:HIS:CE1	1:L:2:LEU:CD2	2.86	0.59
1:I:60:ASN:HB2	1:I:78:TRP:HZ3	1.68	0.59
1:E:18:TRP:CG	1:E:19:PRO:HA	2.38	0.59
1:F:16:ARG:NH2	2:T:1:NAG:C8	2.64	0.59
1:G:35:PRO:HB3	1:G:69:GLY:HA2	1.85	0.58
1:H:16:ARG:HA	1:H:85:ASN:OD1	2.04	0.58
1:C:44:VAL:HG22	1:C:90:TRP:HB3	1.85	0.58
1:J:89:ILE:CD1	1:L:45:SER:HB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LEU:HD21	1:F:4:HIS:NE2	2.17	0.58
1:G:58:ARG:HD3	1:G:78:TRP:NE1	2.18	0.58
1:C:44:VAL:CG1	1:C:45:SER:N	2.67	0.58
1:C:30:ILE:HG21	1:C:90:TRP:CZ2	2.39	0.58
1:I:32:PHE:CD2	1:I:70:GLY:HA2	2.39	0.58
1:C:37:GLU:OE2	1:C:37:GLU:HA	2.04	0.57
1:D:16:ARG:HA	1:D:85:ASN:OD1	2.04	0.57
1:K:42:VAL:HG22	1:K:92:ALA:CB	2.33	0.57
1:E:16:ARG:HA	1:E:85:ASN:OD1	2.05	0.57
1:F:42:VAL:HG22	1:F:92:ALA:CB	2.33	0.57
1:C:7:ARG:O	1:C:93:CYS:HA	2.04	0.57
1:E:50:ASP:HB3	1:E:85:ASN:H	1.69	0.57
1:A:33:TRP:CE3	1:A:34:PRO:HA	2.40	0.57
1:F:32:PHE:CD2	1:F:70:GLY:HA2	2.40	0.57
1:B:3:ILE:HD13	1:E:5:VAL:HG21	1.88	0.56
1:E:75:TYR:OH	1:E:83:VAL:HG21	2.05	0.56
1:D:18:TRP:CG	1:D:19:PRO:HA	2.40	0.56
1:B:62:SER:OG	2:O:1:NAG:H62	2.06	0.56
1:H:18:TRP:CZ2	3:Y:4:A2G:H3	2.40	0.56
1:A:19:PRO:O	1:A:84:TRP:CZ3	2.58	0.56
1:F:75:TYR:HB2	1:F:88:LEU:HD11	1.87	0.56
1:E:75:TYR:CD2	1:E:75:TYR:C	2.78	0.56
1:K:49:LEU:HG	1:K:51:VAL:HG23	1.86	0.56
1:F:12:THR:HG22	1:F:89:ILE:HG22	1.87	0.56
1:A:57:LEU:O	1:B:50:ASP:HA	2.06	0.56
1:G:12:THR:CG2	1:G:89:ILE:HG22	2.35	0.56
1:A:58:ARG:H	1:A:81:THR:HG21	1.72	0.55
1:A:42:VAL:HG22	1:A:92:ALA:HB2	1.88	0.55
1:B:43:ILE:HG13	1:B:43:ILE:O	2.05	0.55
1:B:57:LEU:HD21	1:C:49:LEU:HD23	1.88	0.55
1:B:79:TYR:CE2	1:B:80:THR:HG23	2.42	0.55
1:H:18:TRP:HA	1:H:19:PRO:C	2.27	0.55
1:A:16:ARG:HH22	2:Q:1:NAG:H83	1.71	0.55
1:G:18:TRP:CG	1:G:19:PRO:HA	2.42	0.55
1:K:75:TYR:CG	1:K:76:ASN:N	2.74	0.55
4:A:107:GLA:O4	1:C:58:ARG:NE	2.36	0.55
1:F:58:ARG:HD3	1:F:78:TRP:NE1	2.21	0.55
1:K:42:VAL:HG22	1:K:92:ALA:HB2	1.88	0.54
1:L:49:LEU:HG	1:L:51:VAL:HG23	1.89	0.54
1:E:18:TRP:CD1	1:E:19:PRO:HA	2.43	0.54
1:A:2:LEU:HD23	1:F:4:HIS:CE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:CYS:H	1:B:10:MET:CE	2.20	0.54
1:D:8:CYS:HA	1:D:92:ALA:O	2.07	0.54
1:F:79:TYR:CD1	3:W:4:A2G:C7	2.91	0.54
1:H:3:ILE:HD11	1:K:3:ILE:HD11	1.88	0.54
1:D:60:ASN:ND2	1:D:76:ASN:OD1	2.38	0.54
1:I:58:ARG:HD3	1:I:78:TRP:NE1	2.23	0.54
1:I:32:PHE:O	1:I:33:TRP:CD1	2.52	0.54
1:A:18:TRP:CZ3	4:A:107:GLA:H5	2.43	0.54
1:A:33:TRP:CE3	1:A:35:PRO:HD3	2.43	0.54
1:D:18:TRP:NE1	3:W:3:NGA:O7	2.33	0.53
1:B:18:TRP:CD1	1:B:19:PRO:HA	2.43	0.53
1:D:18:TRP:HB2	1:D:84:TRP:HB3	1.89	0.53
1:F:81:THR:CG2	1:F:82:THR:N	2.71	0.53
1:G:93:CYS:HB2	1:H:10:MET:HE3	1.90	0.53
1:B:17:CYS:HB2	1:B:20:ARG:O	2.09	0.53
1:I:16:ARG:CZ	2:Z:1:NAG:H83	2.39	0.53
1:C:81:THR:HG22	1:C:82:THR:N	2.24	0.53
1:G:2:LEU:HA	1:L:3:ILE:O	2.08	0.53
1:K:75:TYR:CD2	1:K:75:TYR:C	2.81	0.53
1:A:75:TYR:CG	1:A:76:ASN:N	2.74	0.52
1:E:75:TYR:CG	1:E:76:ASN:N	2.75	0.52
1:K:45:SER:HB2	1:L:89:ILE:HD11	1.91	0.52
1:B:43:ILE:HD12	1:C:89:ILE:HD12	1.91	0.52
1:A:45:SER:HB2	1:B:89:ILE:HD11	1.92	0.52
1:D:18:TRP:HA	1:D:19:PRO:C	2.30	0.52
1:D:7:ARG:HD2	1:F:4:HIS:HB2	1.92	0.52
1:H:27:ASP:OD1	1:H:74:HIS:HB2	2.10	0.52
1:G:18:TRP:CD1	1:G:19:PRO:HA	2.45	0.52
1:G:46:PHE:CZ	1:G:59:VAL:HB	2.45	0.52
1:K:18:TRP:CG	1:K:19:PRO:HA	2.45	0.52
1:F:18:TRP:NE1	3:U:3:NGA:O7	2.38	0.52
1:C:1:ARG:HD3	1:D:94:ASP:OD2	2.10	0.51
1:H:38:ASN:C	1:H:68:VAL:HG12	2.31	0.51
1:H:1:ARG:HH22	1:J:4:HIS:H	1.58	0.51
1:K:57:LEU:O	1:L:50:ASP:HA	2.11	0.51
1:J:45:SER:HB2	1:K:89:ILE:CD1	2.40	0.51
1:H:18:TRP:CG	1:H:19:PRO:HA	2.46	0.51
1:I:60:ASN:HB2	1:I:78:TRP:CZ3	2.46	0.51
1:D:50:ASP:HA	1:F:57:LEU:O	2.10	0.51
1:H:3:ILE:O	1:K:2:LEU:HD23	2.09	0.51
1:D:58:ARG:NE	3:S:4:A2G:O6	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:TRP:CD2	1:A:19:PRO:HA	2.45	0.51
1:C:50:ASP:HB3	1:C:85:ASN:N	2.21	0.51
1:L:75:TYR:CG	1:L:76:ASN:N	2.77	0.51
1:E:75:TYR:HB2	1:E:88:LEU:HD11	1.91	0.51
1:G:10:MET:HA	1:G:90:TRP:CZ3	2.45	0.51
1:C:89:ILE:O	1:C:89:ILE:HG13	2.10	0.51
1:C:8:CYS:HA	1:C:92:ALA:O	2.10	0.51
1:G:43:ILE:HG13	1:G:91:ILE:HG22	1.93	0.51
1:A:16:ARG:HA	1:A:85:ASN:OD1	2.11	0.51
1:A:33:TRP:CZ3	1:A:35:PRO:HD3	2.46	0.50
1:F:58:ARG:HB3	1:F:78:TRP:CE3	2.46	0.50
1:I:33:TRP:CD1	1:I:33:TRP:N	2.79	0.50
1:J:89:ILE:HD11	1:L:45:SER:HB2	1.92	0.50
1:A:93:CYS:H	1:B:10:MET:HE3	1.75	0.50
1:F:75:TYR:CD2	1:F:75:TYR:C	2.84	0.50
1:F:79:TYR:OH	3:W:3:NGA:C5	2.59	0.50
1:H:7:ARG:O	1:H:93:CYS:HA	2.12	0.50
1:I:64:ASP:HB2	1:I:72:THR:HB	1.93	0.50
1:A:52:ASP:HA	1:C:56:ASN:CG	2.32	0.50
1:B:91:ILE:O	1:B:91:ILE:HG23	2.10	0.50
1:F:81:THR:HG22	1:F:82:THR:H	1.75	0.50
1:G:51:VAL:HG22	1:G:83:VAL:HG22	1.92	0.50
1:G:48:MET:HB3	1:G:87:LYS:HB3	1.93	0.50
1:J:7:ARG:O	1:J:93:CYS:HA	2.11	0.50
1:L:75:TYR:C	1:L:75:TYR:CD2	2.83	0.50
1:E:58:ARG:H	1:E:81:THR:HG21	1.75	0.50
1:F:58:ARG:HB3	1:F:78:TRP:CE2	2.46	0.50
3:W:1:GAL:O3	3:W:2:GLA:H5	2.12	0.49
1:B:18:TRP:HA	1:B:19:PRO:C	2.33	0.49
1:D:30:ILE:O	1:D:70:GLY:HA3	2.12	0.49
1:B:32:PHE:CD2	1:B:70:GLY:N	2.80	0.49
1:E:58:ARG:HD3	1:E:78:TRP:NE1	2.27	0.49
1:F:32:PHE:CE2	1:F:70:GLY:HA2	2.48	0.49
1:I:17:CYS:O	1:I:18:TRP:C	2.50	0.49
1:B:58:ARG:HD3	1:B:78:TRP:NE1	2.28	0.49
1:G:93:CYS:CB	1:H:10:MET:HE3	2.42	0.49
1:A:52:ASP:HA	1:C:56:ASN:ND2	2.28	0.48
1:J:49:LEU:HG	1:J:51:VAL:HG23	1.94	0.48
1:H:49:LEU:HG	1:H:51:VAL:HG23	1.95	0.48
1:F:79:TYR:OH	3:W:3:NGA:H62	2.13	0.48
1:B:16:ARG:NH1	1:B:16:ARG:HG2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LEU:C	1:D:57:LEU:HD23	2.34	0.48
1:I:32:PHE:CE2	1:I:70:GLY:HA2	2.47	0.48
3:P:1:GAL:O3	3:P:2:GLA:H5	2.12	0.48
1:H:44:VAL:HG22	1:H:90:TRP:HB3	1.95	0.48
1:K:79:TYR:CD2	1:K:80:THR:HG23	2.49	0.48
1:H:58:ARG:HB2	1:H:81:THR:OG1	2.13	0.48
1:I:56:ASN:HB2	1:I:58:ARG:CZ	2.44	0.48
1:H:2:LEU:HD23	1:K:3:ILE:O	2.13	0.48
1:H:79:TYR:CD2	1:H:80:THR:HG23	2.48	0.48
2:Z:1:NAG:H61	2:Z:2:NAG:H82	1.95	0.48
1:A:44:VAL:HG12	1:A:45:SER:N	2.28	0.48
1:A:48:MET:O	1:A:87:LYS:N	2.44	0.48
1:I:58:ARG:NH2	1:I:79:TYR:HD2	2.11	0.48
1:G:40:PRO:HB3	1:G:94:ASP:HB3	1.94	0.48
1:F:79:TYR:OH	3:W:3:NGA:C6	2.62	0.48
1:C:57:LEU:C	1:C:57:LEU:HD23	2.35	0.47
1:F:66:VAL:HG22	1:F:71:PHE:CB	2.44	0.47
1:J:42:VAL:HG22	1:J:92:ALA:CB	2.44	0.47
1:A:91:ILE:HD13	1:B:91:ILE:CD1	2.44	0.47
1:J:45:SER:HB2	1:K:89:ILE:HD11	1.95	0.47
1:C:75:TYR:CD2	1:C:86:TYR:OH	2.67	0.47
1:J:32:PHE:CD2	1:J:70:GLY:HA2	2.49	0.47
1:K:45:SER:HB2	1:L:89:ILE:HD13	1.96	0.47
1:C:18:TRP:NE1	3:P:3:NGA:O7	2.44	0.47
1:G:16:ARG:HA	1:G:85:ASN:OD1	2.14	0.47
1:K:7:ARG:O	1:K:93:CYS:HA	2.14	0.47
1:I:36:PHE:HB3	1:I:38:ASN:O	2.15	0.47
1:A:42:VAL:HG22	1:A:92:ALA:CB	2.44	0.47
1:A:57:LEU:CD1	1:C:57:LEU:HD13	2.45	0.47
1:G:42:VAL:HG22	1:G:92:ALA:HB1	1.96	0.47
1:D:42:VAL:HG22	1:D:92:ALA:CB	2.36	0.47
1:F:7:ARG:NH1	1:F:34:PRO:O	2.41	0.47
1:H:57:LEU:HD13	1:I:57:LEU:CD1	2.45	0.47
1:A:52:ASP:HB2	1:A:84:TRP:NE1	2.26	0.46
1:B:56:ASN:OD1	1:C:52:ASP:HA	2.15	0.46
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.80	0.46
1:D:7:ARG:HD2	1:F:4:HIS:HB3	1.96	0.46
1:G:43:ILE:CG1	1:G:91:ILE:HG22	2.46	0.46
1:E:57:LEU:HD13	1:F:57:LEU:CD1	2.46	0.46
1:B:18:TRP:HA	1:B:20:ARG:N	2.31	0.46
1:A:56:ASN:CG	1:B:52:ASP:HA	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:18:TRP:CD1	1:I:19:PRO:HA	2.50	0.46
1:L:7:ARG:O	1:L:93:CYS:HA	2.15	0.46
1:I:16:ARG:HH22	2:Z:1:NAG:C8	2.29	0.46
1:D:45:SER:HB2	1:E:89:ILE:CD1	2.44	0.45
1:G:50:ASP:HB3	1:G:85:ASN:H	1.81	0.45
1:I:36:PHE:CE2	1:I:94:ASP:HB3	2.50	0.45
1:D:79:TYR:HB2	3:S:4:A2G:O7	2.16	0.45
1:B:7:ARG:O	1:B:93:CYS:HA	2.17	0.45
1:D:56:ASN:CG	1:E:52:ASP:HA	2.36	0.45
1:F:45:SER:OG	1:F:46:PHE:N	2.49	0.45
1:G:89:ILE:O	1:G:89:ILE:HG13	2.16	0.45
1:C:75:TYR:CG	1:C:76:ASN:N	2.82	0.45
1:D:75:TYR:CD2	1:D:86:TYR:OH	2.63	0.45
1:D:41:ASN:O	1:D:92:ALA:HA	2.17	0.45
1:F:66:VAL:HG12	1:F:67:THR:N	2.32	0.45
1:H:1:ARG:NH2	1:J:4:HIS:O	2.50	0.45
1:K:19:PRO:O	1:K:84:TRP:CZ3	2.69	0.45
1:D:79:TYR:CE2	1:D:80:THR:HG23	2.52	0.45
1:D:18:TRP:HE1	3:W:3:NGA:C7	2.28	0.45
1:D:78:TRP:CH2	2:R:1:NAG:H81	2.52	0.45
1:A:91:ILE:HG23	1:A:91:ILE:O	2.17	0.45
1:E:45:SER:HB2	1:F:89:ILE:CD1	2.44	0.45
1:I:36:PHE:CD2	1:I:94:ASP:HB3	2.52	0.45
1:I:58:ARG:HB3	1:I:78:TRP:CE2	2.52	0.45
1:H:18:TRP:CH2	3:Y:4:A2G:H3	2.52	0.45
1:B:84:TRP:CZ2	3:N:3:NGA:H81	2.52	0.44
1:A:89:ILE:O	1:A:89:ILE:HG13	2.16	0.44
1:B:39:THR:HA	1:B:68:VAL:HG12	2.00	0.44
1:C:81:THR:CG2	1:C:82:THR:N	2.80	0.44
3:N:1:GAL:HO6	3:N:2:GLA:C1	2.30	0.44
1:H:41:ASN:O	1:H:92:ALA:HA	2.16	0.44
1:I:52:ASP:HB2	1:I:84:TRP:NE1	2.32	0.44
1:I:1:ARG:HH11	1:I:1:ARG:HG2	1.82	0.44
1:B:89:ILE:O	1:B:89:ILE:HG13	2.17	0.44
1:B:57:LEU:CD2	1:C:49:LEU:HD23	2.47	0.44
1:G:2:LEU:HD22	1:L:2:LEU:HB3	2.00	0.44
1:J:42:VAL:HG22	1:J:92:ALA:HB2	2.00	0.44
1:A:42:VAL:HG12	1:A:43:ILE:N	2.33	0.44
1:D:79:TYR:CD2	1:D:80:THR:HG23	2.52	0.44
1:D:36:PHE:CD2	1:D:94:ASP:HB3	2.53	0.44
1:D:42:VAL:HG12	1:D:43:ILE:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:TYR:CG	1:D:80:THR:N	2.84	0.44
1:E:61:SER:O	1:F:87:LYS:NZ	2.46	0.44
1:K:36:PHE:O	1:K:68:VAL:HB	2.18	0.44
1:H:84:TRP:O	1:H:85:ASN:CG	2.56	0.44
1:D:58:ARG:NH2	3:S:4:A2G:O5	2.51	0.44
1:F:81:THR:CG2	1:F:82:THR:H	2.30	0.43
1:I:1:ARG:N	1:J:5:VAL:O	2.46	0.43
1:C:33:TRP:HA	1:C:34:PRO:HA	1.87	0.43
1:F:41:ASN:O	1:F:92:ALA:HA	2.19	0.43
1:H:2:LEU:HD23	1:H:2:LEU:HA	1.66	0.43
1:H:58:ARG:O	1:H:77:SER:HB2	2.18	0.43
1:I:1:ARG:O	1:J:4:HIS:HA	2.18	0.43
1:H:32:PHE:CE1	1:H:70:GLY:HA2	2.53	0.43
1:E:24:THR:O	1:E:76:ASN:HA	2.18	0.43
1:G:45:SER:HB2	1:H:89:ILE:HD11	2.00	0.43
1:J:16:ARG:HG2	1:J:16:ARG:HH11	1.83	0.43
1:F:79:TYR:OH	3:W:3:NGA:H5	2.17	0.43
1:C:53:ASN:C	1:C:55:ASN:N	2.71	0.43
1:H:91:ILE:HG23	1:H:91:ILE:O	2.19	0.43
1:A:75:TYR:C	1:A:75:TYR:CD2	2.86	0.43
1:G:42:VAL:HG22	1:G:92:ALA:HB2	1.98	0.43
1:I:89:ILE:O	1:I:89:ILE:HG13	2.19	0.43
1:C:16:ARG:HB3	1:C:16:ARG:HH11	1.84	0.43
1:D:81:THR:HG22	1:D:82:THR:N	2.33	0.43
1:G:48:MET:HE1	1:G:86:TYR:N	2.34	0.43
1:A:48:MET:O	1:A:86:TYR:CA	2.65	0.43
1:A:3:ILE:HB	1:E:1:ARG:NH2	2.34	0.43
1:E:62:SER:OG	1:E:63:ALA:N	2.52	0.43
1:H:5:VAL:O	1:K:1:ARG:N	2.41	0.43
1:I:42:VAL:HG22	1:I:92:ALA:HB2	2.01	0.43
1:K:12:THR:HG22	1:K:89:ILE:HG22	2.01	0.43
1:I:42:VAL:HG22	1:I:92:ALA:CB	2.48	0.43
1:C:2:LEU:HG	1:D:4:HIS:CE1	2.54	0.42
1:E:39:THR:N	1:E:68:VAL:HG12	2.34	0.42
1:F:49:LEU:HA	1:F:49:LEU:HD12	1.83	0.42
1:G:22:CYS:SG	1:G:83:VAL:O	2.77	0.42
1:I:16:ARG:NH1	2:Z:1:NAG:C8	2.64	0.42
1:L:32:PHE:CD2	1:L:70:GLY:HA2	2.55	0.42
1:A:58:ARG:HG3	1:A:81:THR:OG1	2.19	0.42
1:B:61:SER:HA	1:B:74:HIS:O	2.18	0.42
1:C:18:TRP:CZ2	3:P:4:A2G:H3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:VAL:HG22	1:D:71:PHE:HB2	2.01	0.42
1:E:44:VAL:HG12	1:E:45:SER:N	2.35	0.42
1:B:33:TRP:HA	1:B:34:PRO:C	2.40	0.42
1:A:84:TRP:HD1	4:A:107:GLA:HO6	1.54	0.42
1:B:17:CYS:CB	1:B:20:ARG:O	2.67	0.42
1:I:2:LEU:HB3	1:J:2:LEU:HD22	2.01	0.42
1:K:59:VAL:O	1:L:48:MET:HG2	2.20	0.42
1:A:16:ARG:NH1	1:A:16:ARG:HG2	2.35	0.42
1:A:36:PHE:CD2	1:A:94:ASP:HB3	2.55	0.42
1:K:32:PHE:CD2	1:K:70:GLY:HA2	2.55	0.42
1:L:18:TRP:CG	1:L:19:PRO:HA	2.48	0.42
1:I:75:TYR:CG	1:I:76:ASN:N	2.87	0.42
1:J:36:PHE:O	1:J:68:VAL:HB	2.19	0.42
1:C:35:PRO:HB3	1:C:68:VAL:O	2.20	0.41
1:D:50:ASP:HB3	1:D:85:ASN:H	1.85	0.41
1:L:42:VAL:HG22	1:L:92:ALA:CB	2.49	0.41
1:E:56:ASN:CG	1:F:52:ASP:HA	2.41	0.41
1:A:24:THR:O	1:A:76:ASN:HA	2.21	0.41
1:B:75:TYR:CG	1:B:76:ASN:N	2.86	0.41
1:H:45:SER:HB2	1:I:89:ILE:HD13	2.00	0.41
1:H:75:TYR:CD2	1:H:75:TYR:C	2.93	0.41
1:G:79:TYR:CZ	3:Y:3:NGA:H4	2.55	0.41
1:I:44:VAL:HG11	1:I:73:LEU:HD11	2.03	0.41
1:I:48:MET:O	1:I:86:TYR:HA	2.20	0.41
1:J:89:ILE:HD13	1:L:45:SER:HB2	2.00	0.41
1:G:3:ILE:CD1	1:L:5:VAL:HG21	2.50	0.41
1:K:58:ARG:HD3	1:K:78:TRP:NE1	2.36	0.41
1:F:6:SER:HA	1:F:94:ASP:O	2.21	0.41
1:G:36:PHE:O	1:G:68:VAL:HB	2.21	0.41
1:B:3:ILE:CD1	1:E:5:VAL:HG21	2.49	0.41
1:G:85:ASN:O	1:G:86:TYR:HB3	2.20	0.41
1:H:12:THR:HG22	1:H:89:ILE:HG22	2.01	0.41
1:I:49:LEU:HD11	1:I:59:VAL:HG11	2.03	0.41
1:K:19:PRO:O	1:K:84:TRP:HZ3	2.03	0.41
1:B:16:ARG:HA	1:B:85:ASN:OD1	2.20	0.41
1:D:89:ILE:HG13	1:D:89:ILE:O	2.19	0.41
1:A:79:TYR:CE2	1:A:80:THR:HG23	2.56	0.41
1:C:49:LEU:HG	1:C:51:VAL:HG23	2.02	0.41
1:E:79:TYR:OH	3:U:3:NGA:H5	2.20	0.41
1:H:33:TRP:HA	1:H:34:PRO:HA	1.85	0.41
1:B:79:TYR:HB2	3:P:4:A2G:O7	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:TYR:OH	1:D:83:VAL:HG21	2.21	0.41
1:E:45:SER:OG	1:E:46:PHE:N	2.54	0.41
1:I:33:TRP:HA	1:I:34:PRO:HA	1.82	0.41
1:A:75:TYR:OH	1:A:83:VAL:HG21	2.21	0.41
1:C:16:ARG:HA	1:C:85:ASN:OD1	2.20	0.41
1:C:18:TRP:CG	1:C:19:PRO:HA	2.52	0.41
1:G:64:ASP:HB2	1:G:72:THR:HB	2.02	0.41
1:H:84:TRP:CD1	3:Y:4:A2G:H14	2.56	0.41
1:I:28:GLU:HG3	1:I:29:PRO:HD2	2.03	0.40
1:G:49:LEU:HD11	1:G:59:VAL:HG11	2.02	0.40
1:E:79:TYR:CZ	3:U:3:NGA:H4	2.56	0.40
1:B:16:ARG:HH11	1:B:16:ARG:HG2	1.86	0.40
1:E:49:LEU:HD11	1:E:59:VAL:HG11	2.03	0.40
1:L:1:ARG:HG3	1:L:3:ILE:HG23	2.02	0.40
1:B:91:ILE:O	1:B:91:ILE:CG2	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
1	B	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
1	C	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
1	D	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
1	E	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
1	F	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
1	G	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
1	H	92/94 (98%)	83 (90%)	8 (9%)	1 (1%)	14	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
1	J	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	K	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	L	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
All	All	1104/1128 (98%)	1049 (95%)	54 (5%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	19	PRO

### 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	88/88 (100%)	87 (99%)	1 (1%)	73	86
1	B	87/88 (99%)	87 (100%)	0	100	100
1	C	88/88 (100%)	88 (100%)	0	100	100
1	D	87/88 (99%)	87 (100%)	0	100	100
1	E	88/88 (100%)	88 (100%)	0	100	100
1	F	88/88 (100%)	88 (100%)	0	100	100
1	G	88/88 (100%)	88 (100%)	0	100	100
1	H	88/88 (100%)	88 (100%)	0	100	100
1	I	87/88 (99%)	87 (100%)	0	100	100
1	J	87/88 (99%)	87 (100%)	0	100	100
1	K	87/88 (99%)	86 (99%)	1 (1%)	73	86
1	L	85/88 (97%)	84 (99%)	1 (1%)	71	85
All	All	1048/1056 (99%)	1045 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	K	1	ARG
1	L	1	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	4	HIS
1	E	4	HIS
1	G	4	HIS
1	L	4	HIS
1	L	38	ASN

### 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](#)

64 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	M	1	1,2	14,14,15	0.48	0	17,19,21	0.81	0
2	NAG	M	2	2	14,14,15	0.50	0	17,19,21	0.66	0
3	GAL	N	1	3	12,12,12	0.70	0	17,17,17	0.57	0
3	GLA	N	2	3	11,11,12	0.71	0	15,15,17	0.70	0
3	NGA	N	3	3	14,14,15	0.75	0	17,19,21	0.65	0
3	A2G	N	4	3	14,14,15	0.41	0	17,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	O	1	1,2	14,14,15	0.53	0	17,19,21	0.58	0
2	NAG	O	2	2	14,14,15	0.60	0	17,19,21	0.54	0
3	GAL	P	1	3	12,12,12	0.73	0	17,17,17	0.58	0
3	GLA	P	2	3	11,11,12	0.72	0	15,15,17	0.68	0
3	NGA	P	3	3	14,14,15	0.68	0	17,19,21	0.68	0
3	A2G	P	4	3	14,14,15	0.43	0	17,19,21	0.79	0
2	NAG	Q	1	1,2	14,14,15	0.50	0	17,19,21	0.75	0
2	NAG	Q	2	2	14,14,15	0.48	0	17,19,21	0.54	0
2	NAG	R	1	1,2	14,14,15	0.42	0	17,19,21	0.79	0
2	NAG	R	2	2	14,14,15	0.56	0	17,19,21	0.66	0
3	GAL	S	1	3	12,12,12	0.70	0	17,17,17	0.56	0
3	GLA	S	2	3	11,11,12	0.67	0	15,15,17	0.68	0
3	NGA	S	3	3	14,14,15	0.72	0	17,19,21	0.56	0
3	A2G	S	4	3	14,14,15	0.48	0	17,19,21	0.78	0
2	NAG	T	1	1,2	14,14,15	0.65	0	17,19,21	0.96	0
2	NAG	T	2	2	14,14,15	0.63	0	17,19,21	0.63	0
3	GAL	U	1	3	12,12,12	0.68	0	17,17,17	0.57	0
3	GLA	U	2	3	11,11,12	0.70	0	15,15,17	0.68	0
3	NGA	U	3	3	14,14,15	0.71	0	17,19,21	0.56	0
3	A2G	U	4	3	14,14,15	0.48	0	17,19,21	0.79	0
2	NAG	V	1	1,2	14,14,15	0.54	0	17,19,21	0.80	0
2	NAG	V	2	2	14,14,15	0.63	0	17,19,21	0.73	0
3	GAL	W	1	3	12,12,12	0.74	0	17,17,17	0.60	0
3	GLA	W	2	3	11,11,12	0.69	0	15,15,17	0.68	0
3	NGA	W	3	3	14,14,15	0.67	0	17,19,21	0.58	0
3	A2G	W	4	3	14,14,15	0.44	0	17,19,21	0.78	0
2	NAG	X	1	1,2	14,14,15	0.50	0	17,19,21	0.74	0
2	NAG	X	2	2	14,14,15	0.59	0	17,19,21	0.57	0
3	GAL	Y	1	3	12,12,12	0.68	0	17,17,17	0.56	0
3	GLA	Y	2	3	11,11,12	0.70	0	15,15,17	0.69	0
3	NGA	Y	3	3	14,14,15	0.68	0	17,19,21	0.56	0
3	A2G	Y	4	3	14,14,15	0.42	0	17,19,21	0.80	0
2	NAG	Z	1	1,2	14,14,15	0.59	0	17,19,21	0.66	0
2	NAG	Z	2	2	14,14,15	0.52	0	17,19,21	0.50	0
3	GAL	a	1	3	12,12,12	0.40	0	17,17,17	0.43	0
3	GLA	a	2	3	11,11,12	0.54	0	15,15,17	0.91	0
3	NGA	a	3	3	14,14,15	0.55	0	17,19,21	0.54	0
3	A2G	a	4	3	14,14,15	0.50	0	17,19,21	0.65	0
2	NAG	b	1	1,2	14,14,15	0.64	0	17,19,21	0.50	0
2	NAG	b	2	2	14,14,15	0.50	0	17,19,21	0.53	0
2	NAG	c	1	1,2	14,14,15	0.52	0	17,19,21	0.49	0
2	NAG	c	2	2	14,14,15	0.53	0	17,19,21	0.50	0
3	GAL	d	1	3	12,12,12	0.74	0	17,17,17	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLA	d	2	3	11,11,12	0.70	0	15,15,17	0.68	0
3	NGA	d	3	3	14,14,15	0.74	0	17,19,21	0.55	0
3	A2G	d	4	3	14,14,15	0.44	0	17,19,21	0.79	0
2	NAG	e	1	1,2	14,14,15	0.53	0	17,19,21	0.51	0
2	NAG	e	2	2	14,14,15	0.50	0	17,19,21	0.52	0
3	GAL	f	1	3	12,12,12	0.71	0	17,17,17	0.56	0
3	GLA	f	2	3	11,11,12	0.70	0	15,15,17	0.69	0
3	NGA	f	3	3	14,14,15	0.72	0	17,19,21	0.56	0
3	A2G	f	4	3	14,14,15	0.46	0	17,19,21	0.78	0
2	NAG	g	1	1,2	14,14,15	0.67	0	17,19,21	0.70	0
2	NAG	g	2	2	14,14,15	0.51	0	17,19,21	0.57	0
3	GAL	h	1	3	12,12,12	0.71	0	17,17,17	0.57	0
3	GLA	h	2	3	11,11,12	0.66	0	15,15,17	0.69	0
3	NGA	h	3	3	14,14,15	0.71	0	17,19,21	0.56	0
3	A2G	h	4	3	14,14,15	0.45	0	17,19,21	0.78	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
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
3	GAL	N	1	3	-	0/2/22/22	0/1/1/1
3	GLA	N	2	3	-	0/2/19/22	0/1/1/1
3	NGA	N	3	3	-	0/6/23/26	0/1/1/1
3	A2G	N	4	3	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	4/6/23/26	0/1/1/1
3	GAL	P	1	3	-	0/2/22/22	0/1/1/1
3	GLA	P	2	3	-	0/2/19/22	0/1/1/1
3	NGA	P	3	3	-	0/6/23/26	0/1/1/1
3	A2G	P	4	3	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	4/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
3	GAL	S	1	3	-	2/2/22/22	0/1/1/1
3	GLA	S	2	3	-	0/2/19/22	0/1/1/1
3	NGA	S	3	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2G	S	4	3	-	2/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	4/6/23/26	0/1/1/1
3	GAL	U	1	3	-	0/2/22/22	0/1/1/1
3	GLA	U	2	3	-	0/2/19/22	0/1/1/1
3	NGA	U	3	3	-	0/6/23/26	0/1/1/1
3	A2G	U	4	3	-	2/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	4/6/23/26	0/1/1/1
3	GAL	W	1	3	-	0/2/22/22	0/1/1/1
3	GLA	W	2	3	-	0/2/19/22	0/1/1/1
3	NGA	W	3	3	-	0/6/23/26	0/1/1/1
3	A2G	W	4	3	-	2/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	X	2	2	-	4/6/23/26	0/1/1/1
3	GAL	Y	1	3	-	0/2/22/22	0/1/1/1
3	GLA	Y	2	3	-	0/2/19/22	0/1/1/1
3	NGA	Y	3	3	-	0/6/23/26	0/1/1/1
3	A2G	Y	4	3	-	2/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/23/26	0/1/1/1
3	GAL	a	1	3	-	1/2/22/22	0/1/1/1
3	GLA	a	2	3	-	2/2/19/22	0/1/1/1
3	NGA	a	3	3	-	3/6/23/26	0/1/1/1
3	A2G	a	4	3	-	4/6/23/26	0/1/1/1
2	NAG	b	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	4/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	c	2	2	-	4/6/23/26	0/1/1/1
3	GAL	d	1	3	-	2/2/22/22	0/1/1/1
3	GLA	d	2	3	-	0/2/19/22	0/1/1/1
3	NGA	d	3	3	-	0/6/23/26	0/1/1/1
3	A2G	d	4	3	-	2/6/23/26	0/1/1/1
2	NAG	e	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	4/6/23/26	0/1/1/1
3	GAL	f	1	3	-	0/2/22/22	0/1/1/1
3	GLA	f	2	3	-	0/2/19/22	0/1/1/1
3	NGA	f	3	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2G	f	4	3	-	2/6/23/26	0/1/1/1
2	NAG	g	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	g	2	2	-	4/6/23/26	0/1/1/1
3	GAL	h	1	3	-	0/2/22/22	0/1/1/1
3	GLA	h	2	3	-	0/2/19/22	0/1/1/1
3	NGA	h	3	3	-	0/6/23/26	0/1/1/1
3	A2G	h	4	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	2	NAG	C8-C7-N2-C2
2	V	2	NAG	O7-C7-N2-C2
2	b	2	NAG	C8-C7-N2-C2
2	b	2	NAG	O7-C7-N2-C2
2	T	2	NAG	C8-C7-N2-C2
2	T	2	NAG	O7-C7-N2-C2
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
2	c	2	NAG	C8-C7-N2-C2
2	c	2	NAG	O7-C7-N2-C2
2	e	2	NAG	C8-C7-N2-C2
2	e	2	NAG	O7-C7-N2-C2
2	g	2	NAG	C8-C7-N2-C2
2	g	2	NAG	O7-C7-N2-C2
2	X	2	NAG	C8-C7-N2-C2
2	X	2	NAG	O7-C7-N2-C2
2	O	2	NAG	C8-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2
2	Q	2	NAG	C8-C7-N2-C2
2	Q	2	NAG	O7-C7-N2-C2
2	Z	2	NAG	C8-C7-N2-C2
2	Z	2	NAG	O7-C7-N2-C2
3	d	1	GAL	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
3	a	4	A2G	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	d	1	GAL	C4-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
3	a	3	NGA	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
3	f	4	A2G	O5-C5-C6-O6
3	W	4	A2G	O5-C5-C6-O6
3	U	4	A2G	O5-C5-C6-O6
3	N	4	A2G	O5-C5-C6-O6
3	S	4	A2G	O5-C5-C6-O6
3	h	4	A2G	O5-C5-C6-O6
3	Y	4	A2G	O5-C5-C6-O6
3	P	4	A2G	O5-C5-C6-O6
3	d	4	A2G	O5-C5-C6-O6
3	a	3	NGA	C4-C5-C6-O6
3	a	4	A2G	O7-C7-N2-C2
3	a	4	A2G	C8-C7-N2-C2
2	T	2	NAG	C4-C5-C6-O6
3	N	4	A2G	C4-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
2	c	2	NAG	O5-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
3	f	4	A2G	C4-C5-C6-O6
3	W	4	A2G	C4-C5-C6-O6
3	U	4	A2G	C4-C5-C6-O6
3	S	4	A2G	C4-C5-C6-O6
3	h	4	A2G	C4-C5-C6-O6
3	P	4	A2G	C4-C5-C6-O6
3	d	4	A2G	C4-C5-C6-O6
3	a	2	GLA	O5-C5-C6-O6
2	e	2	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6
3	Y	4	A2G	C4-C5-C6-O6
3	a	2	GLA	C4-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
3	a	4	A2G	C4-C5-C6-O6
3	a	1	GAL	O5-C5-C6-O6
2	c	2	NAG	C4-C5-C6-O6
2	b	2	NAG	C4-C5-C6-O6
2	e	2	NAG	C4-C5-C6-O6

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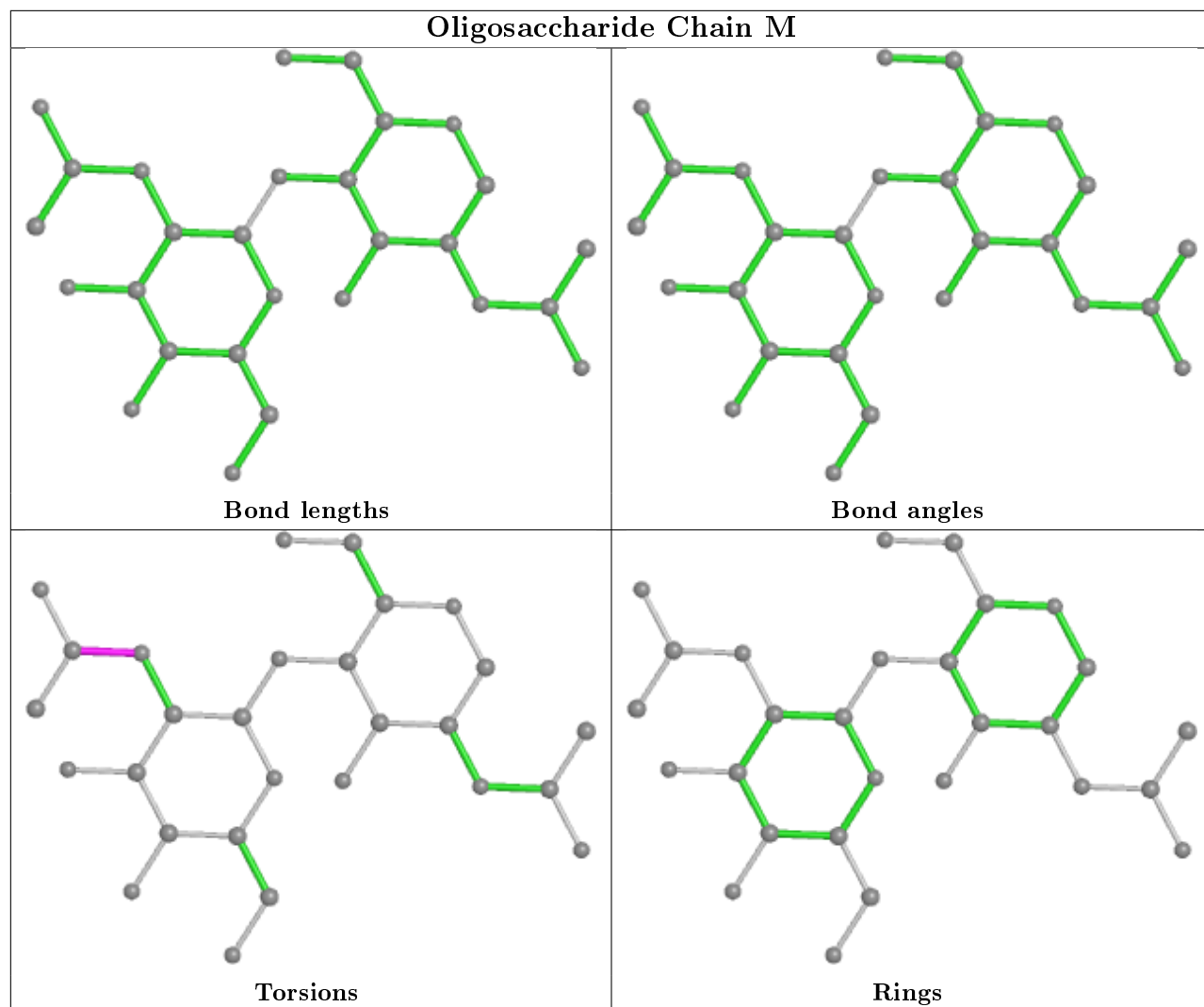
Mol	Chain	Res	Type	Atoms
2	g	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	R	2	NAG	C8-C7-N2-C2
3	S	1	GAL	C4-C5-C6-O6
2	R	2	NAG	O7-C7-N2-C2
2	V	2	NAG	C4-C5-C6-O6
3	a	3	NGA	C3-C2-N2-C7
3	S	1	GAL	O5-C5-C6-O6

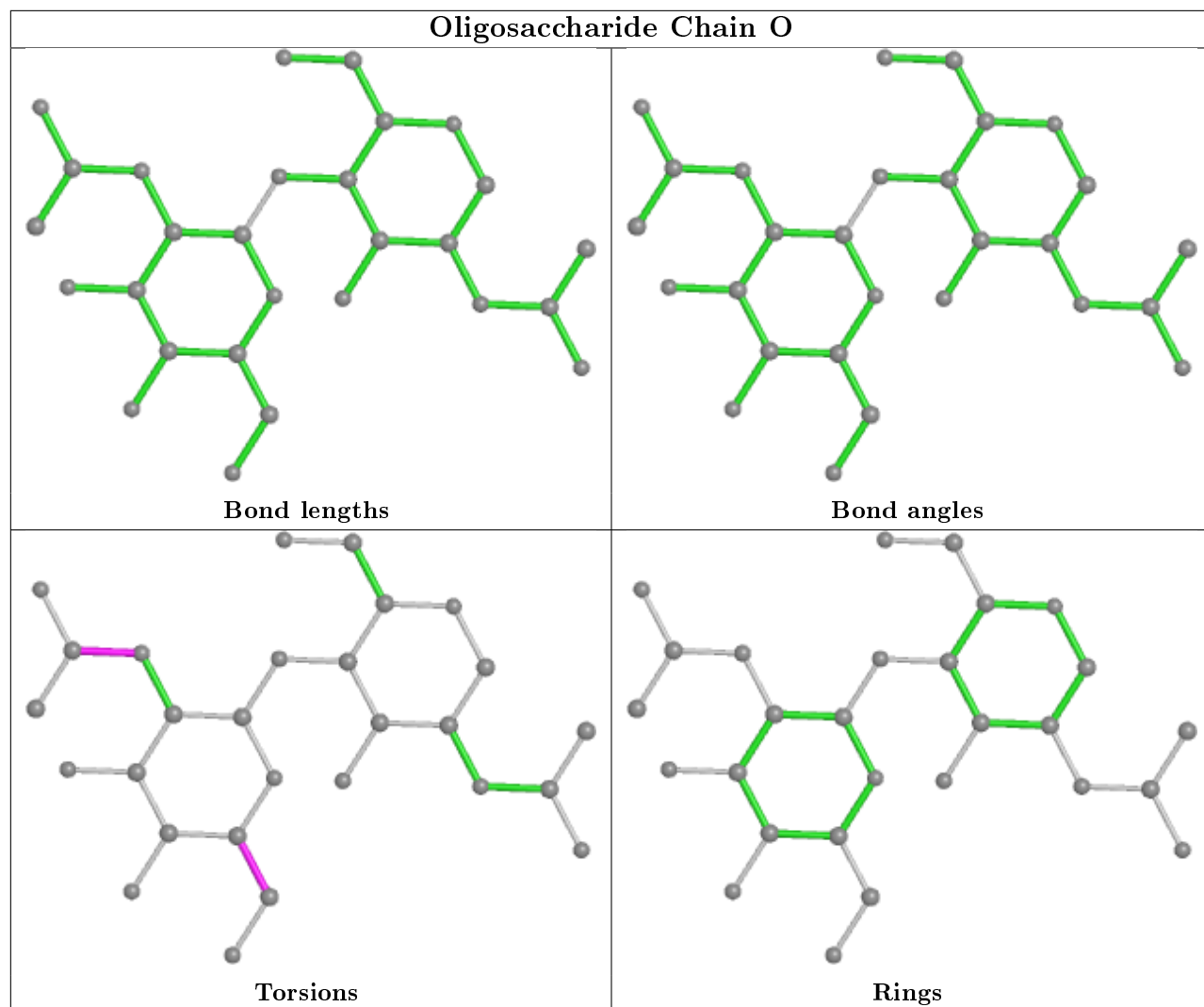
There are no ring outliers.

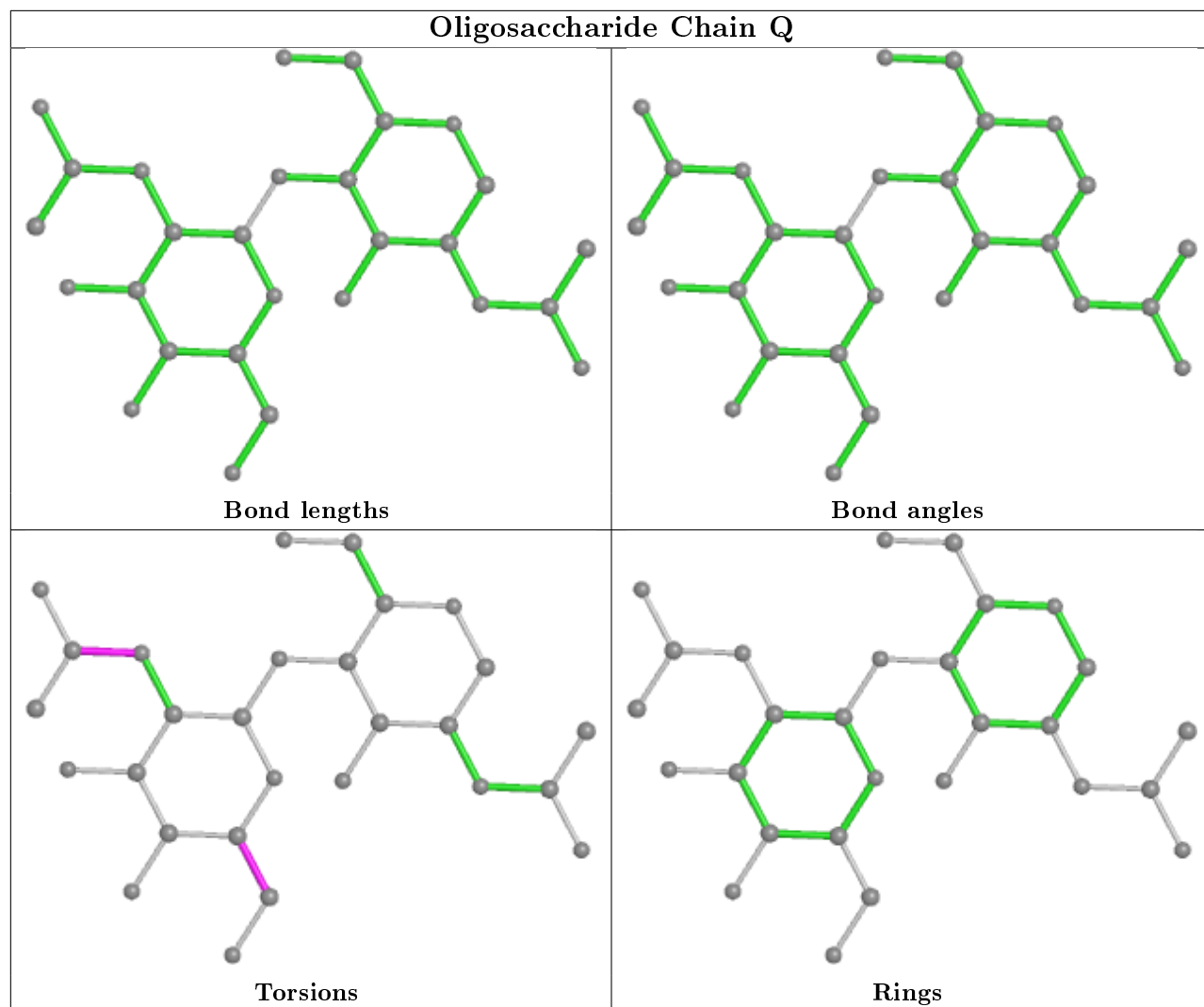
25 monomers are involved in 56 short contacts:

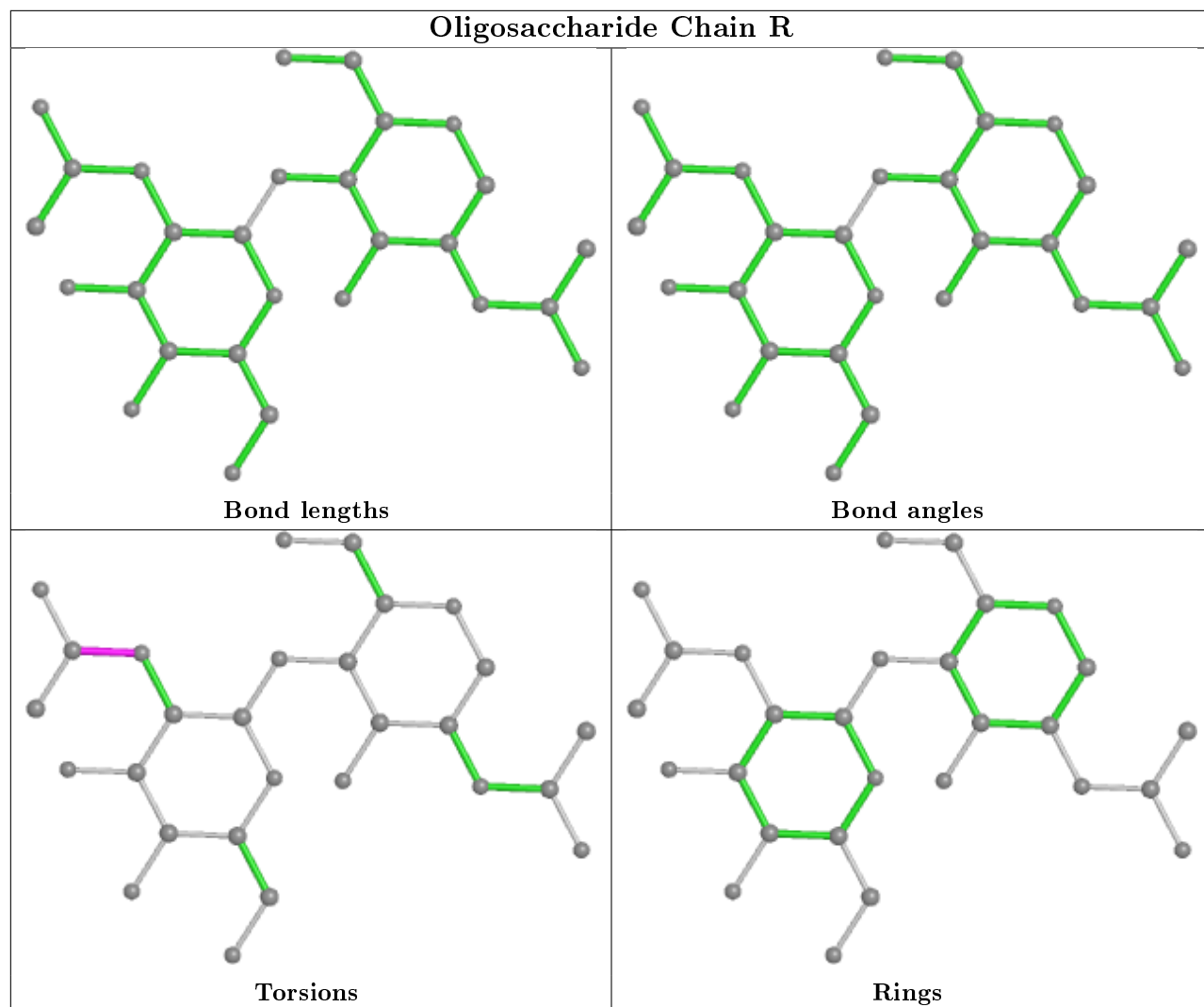
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	1	NAG	1	0
3	W	2	GLA	1	0
3	U	3	NGA	3	0
3	W	4	A2G	1	0
3	N	2	GLA	1	0
2	O	1	NAG	1	0
2	T	1	NAG	4	0
2	X	1	NAG	5	0
3	N	3	NGA	1	0
3	P	3	NGA	1	0
3	N	1	GAL	1	0
3	Y	3	NGA	1	0
3	N	4	A2G	1	0
3	S	4	A2G	3	0
2	Z	2	NAG	1	0
2	Z	1	NAG	8	0
2	M	1	NAG	1	0
2	R	1	NAG	6	0
3	W	1	GAL	1	0
3	P	1	GAL	1	0
3	Y	4	A2G	4	0
3	P	4	A2G	2	0
3	W	3	NGA	7	0
3	P	2	GLA	1	0
2	V	1	NAG	3	0

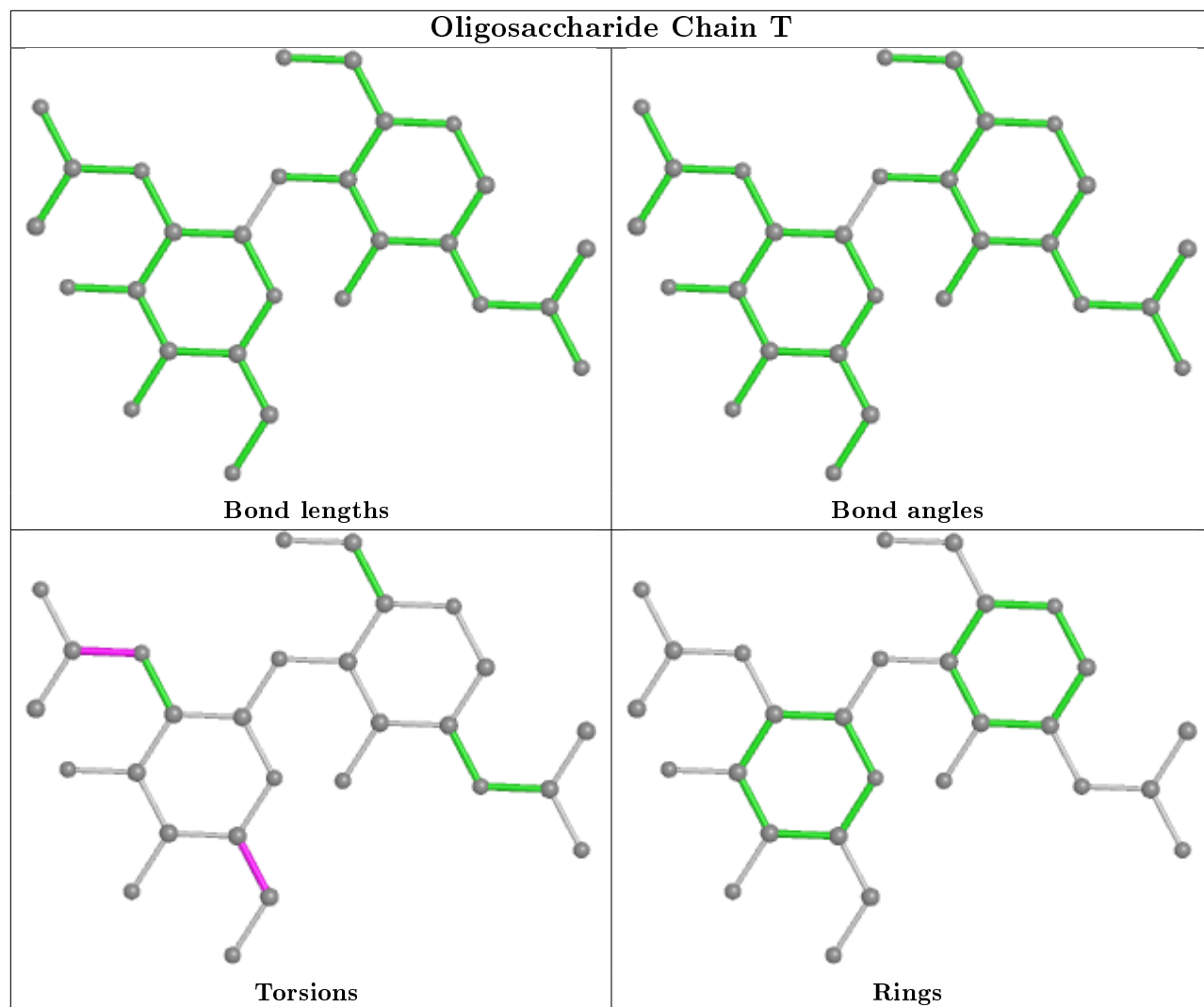
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



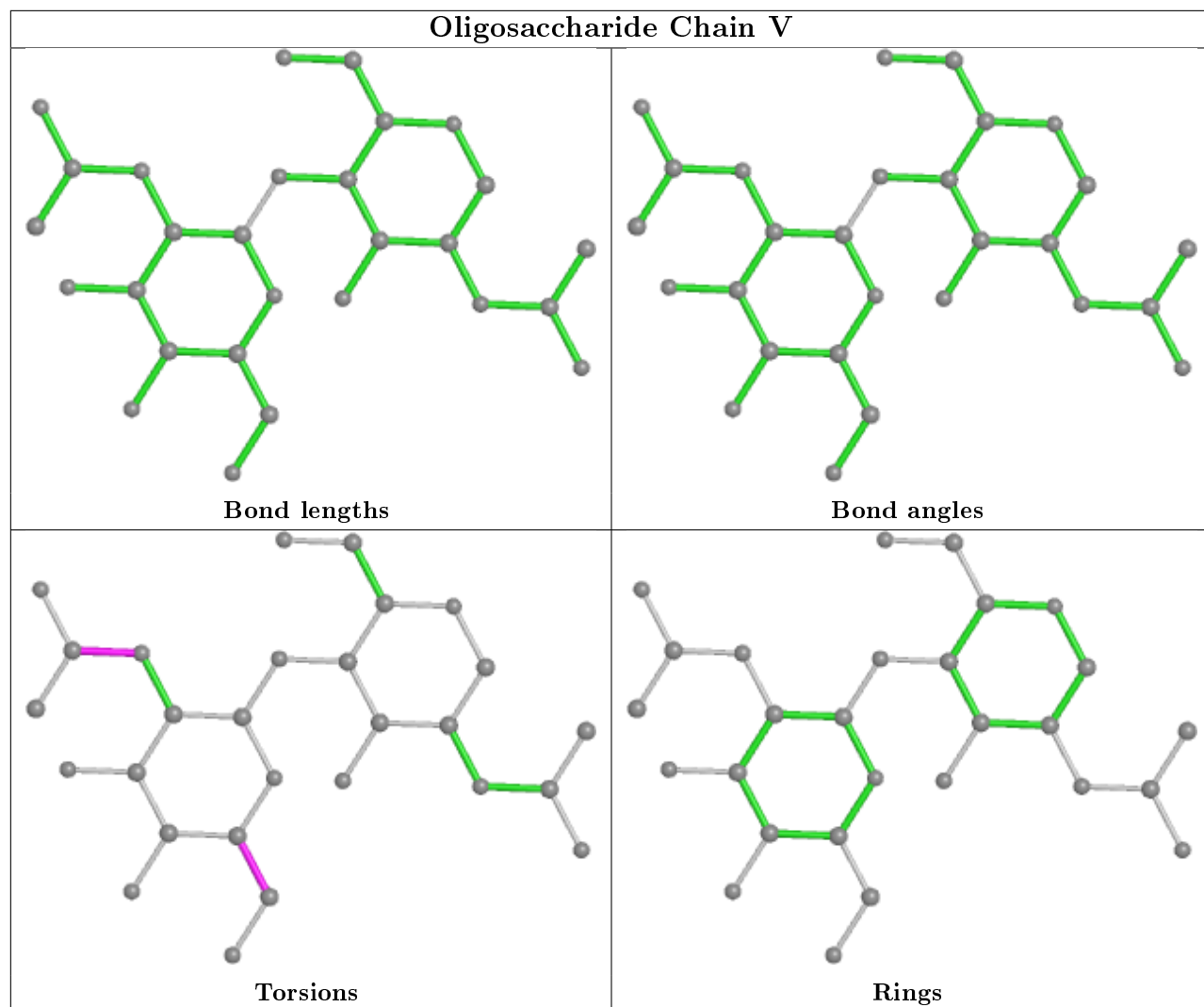


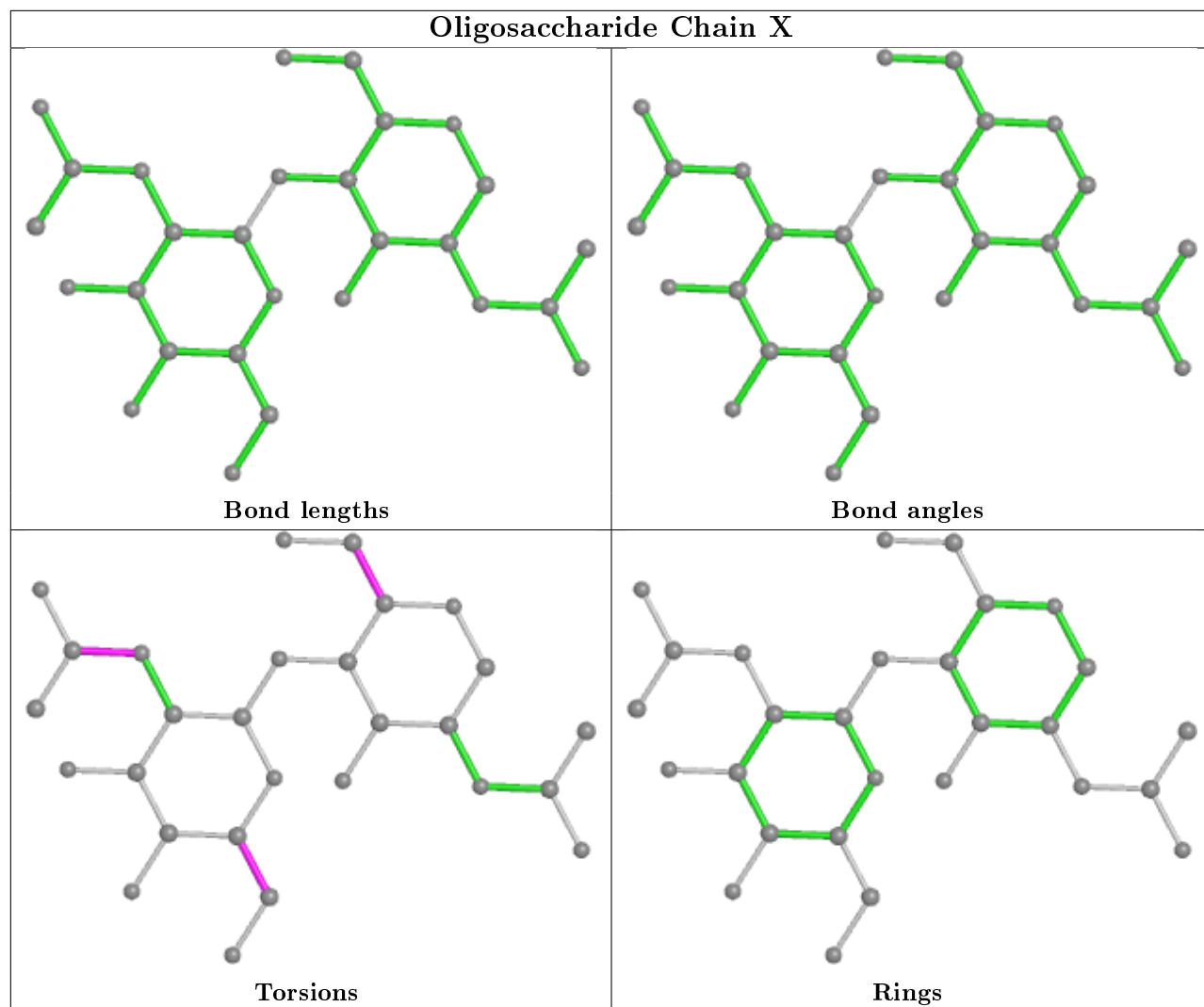


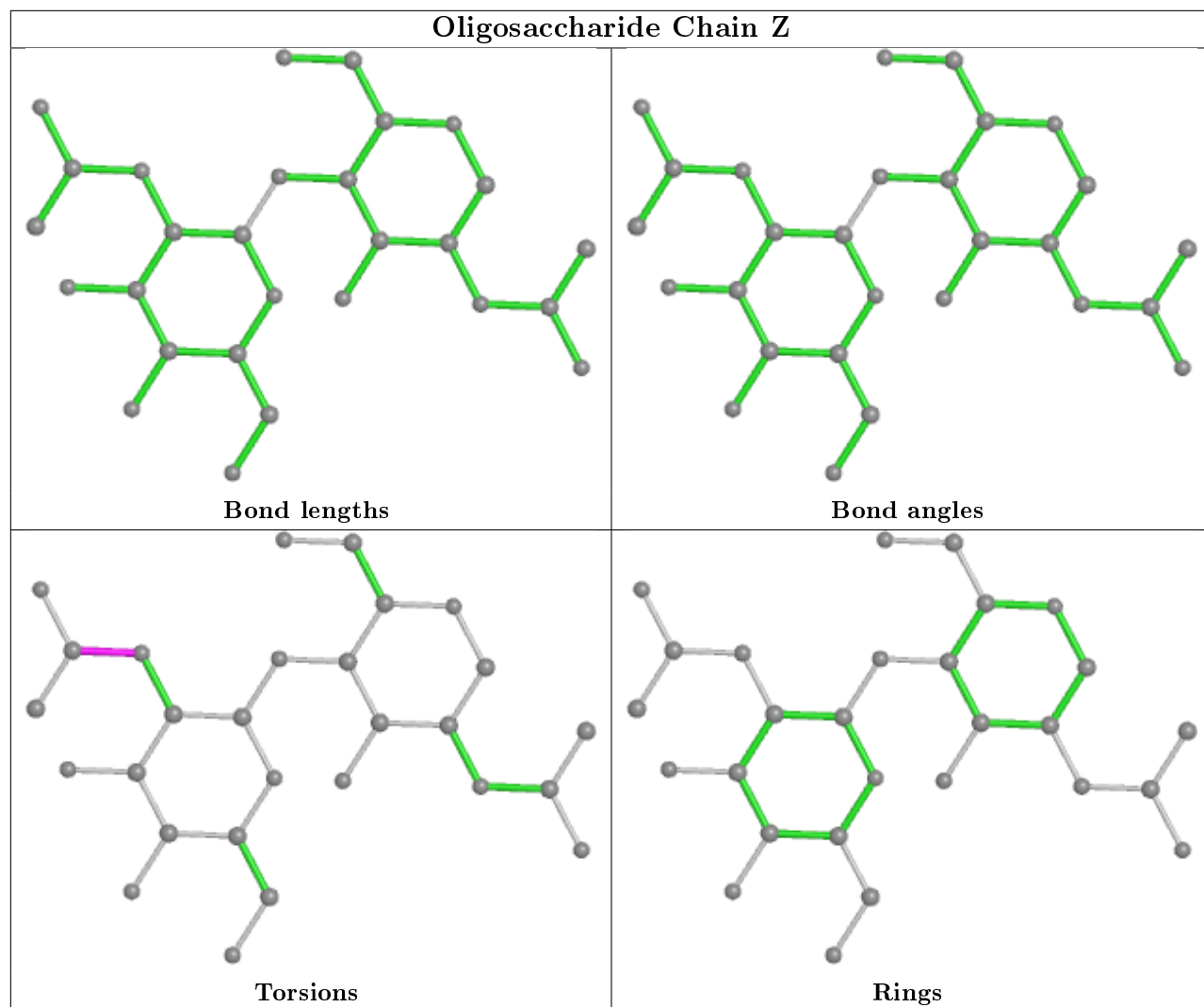


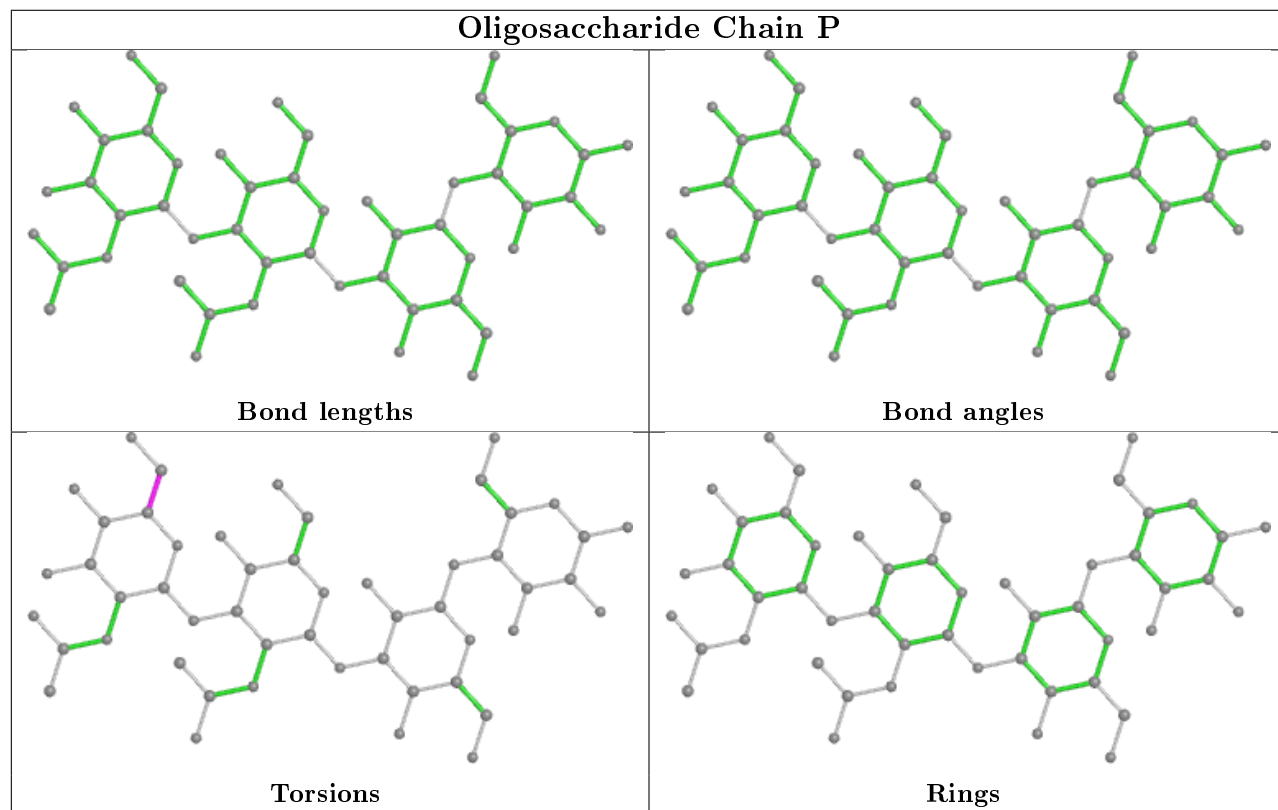
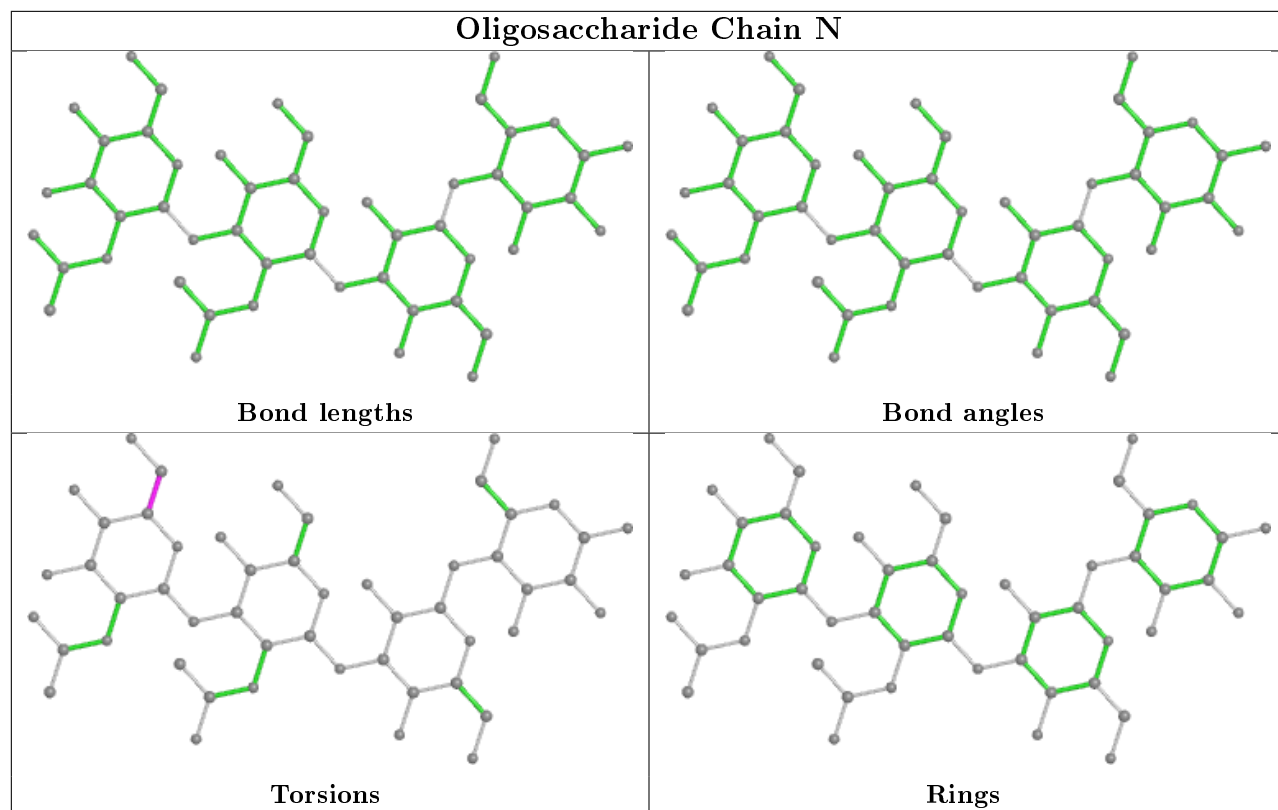


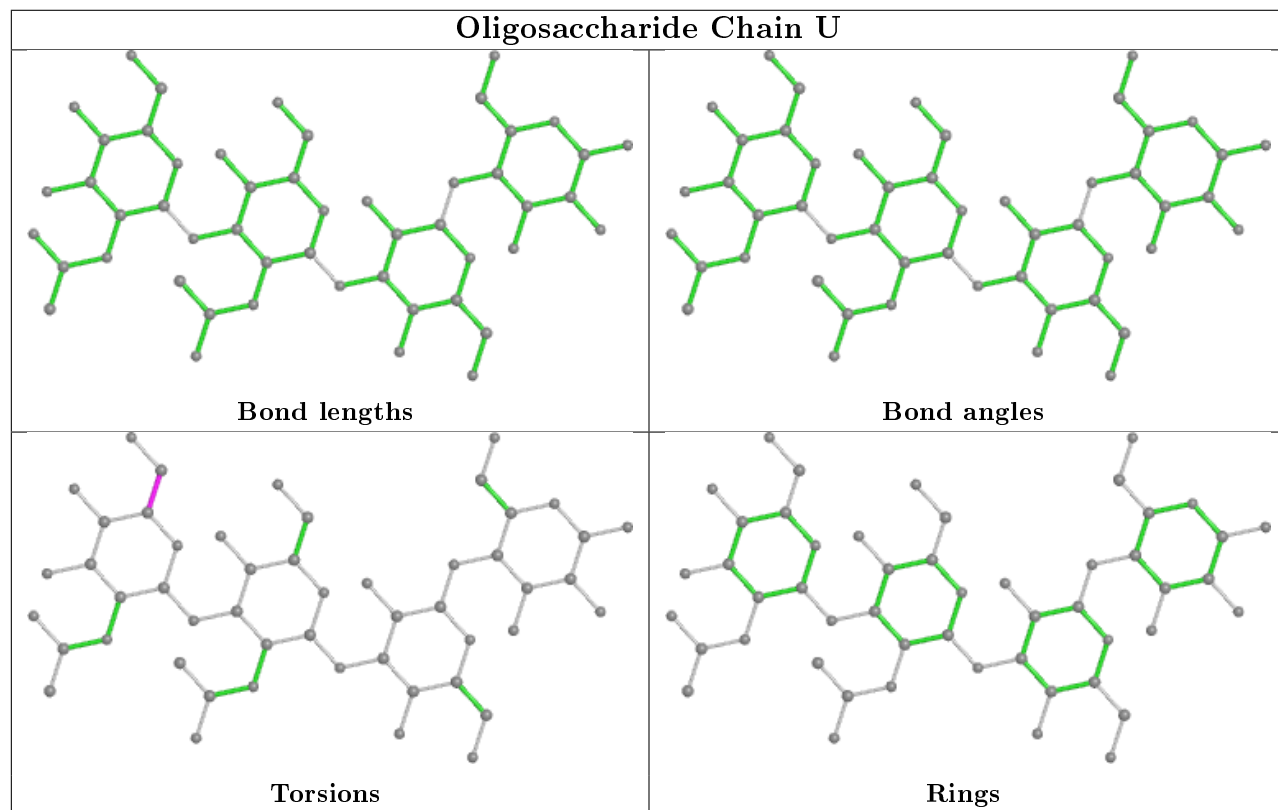
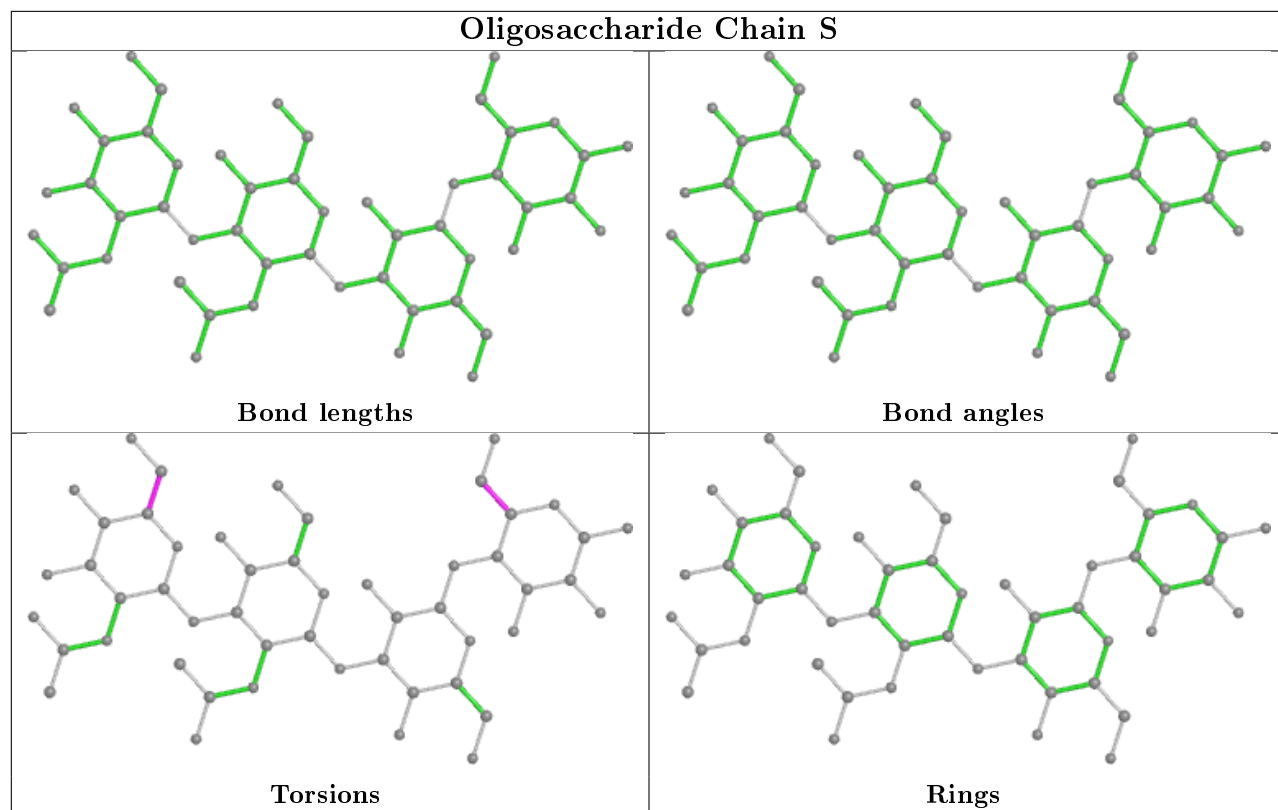


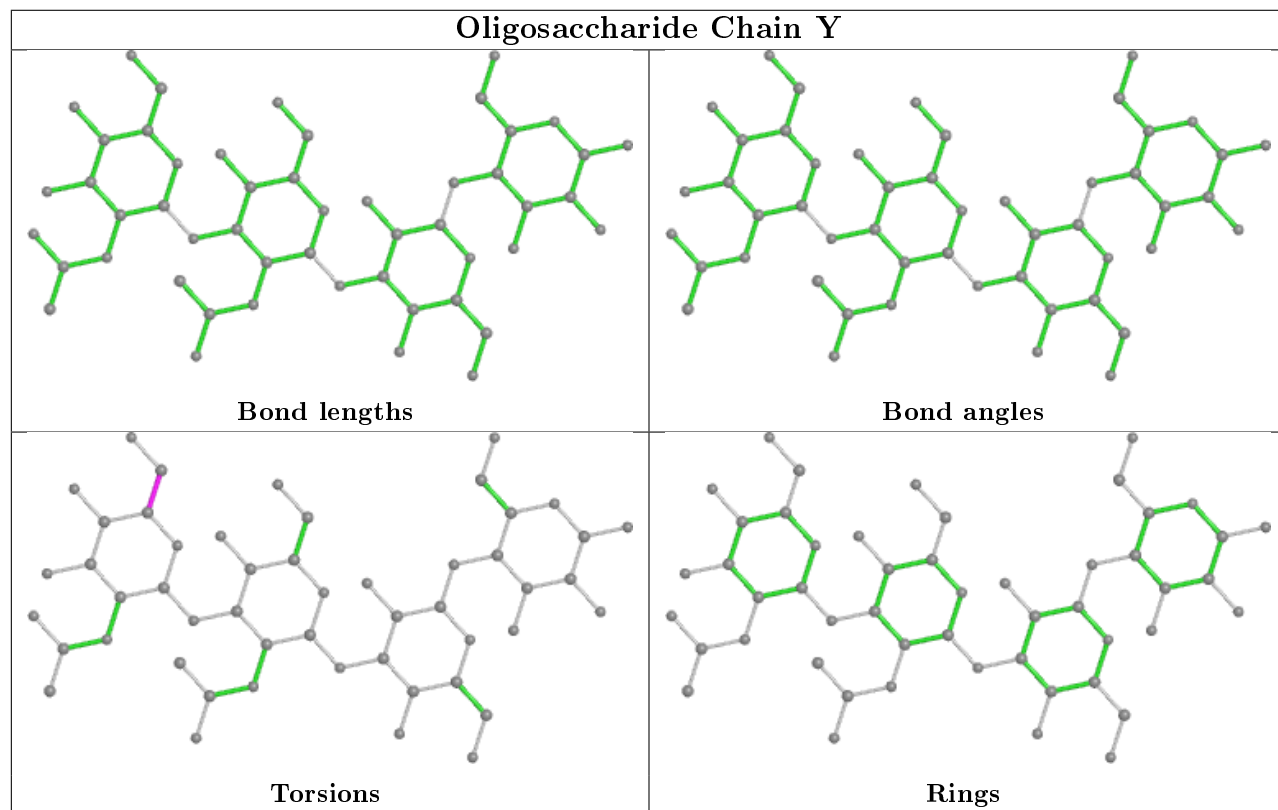
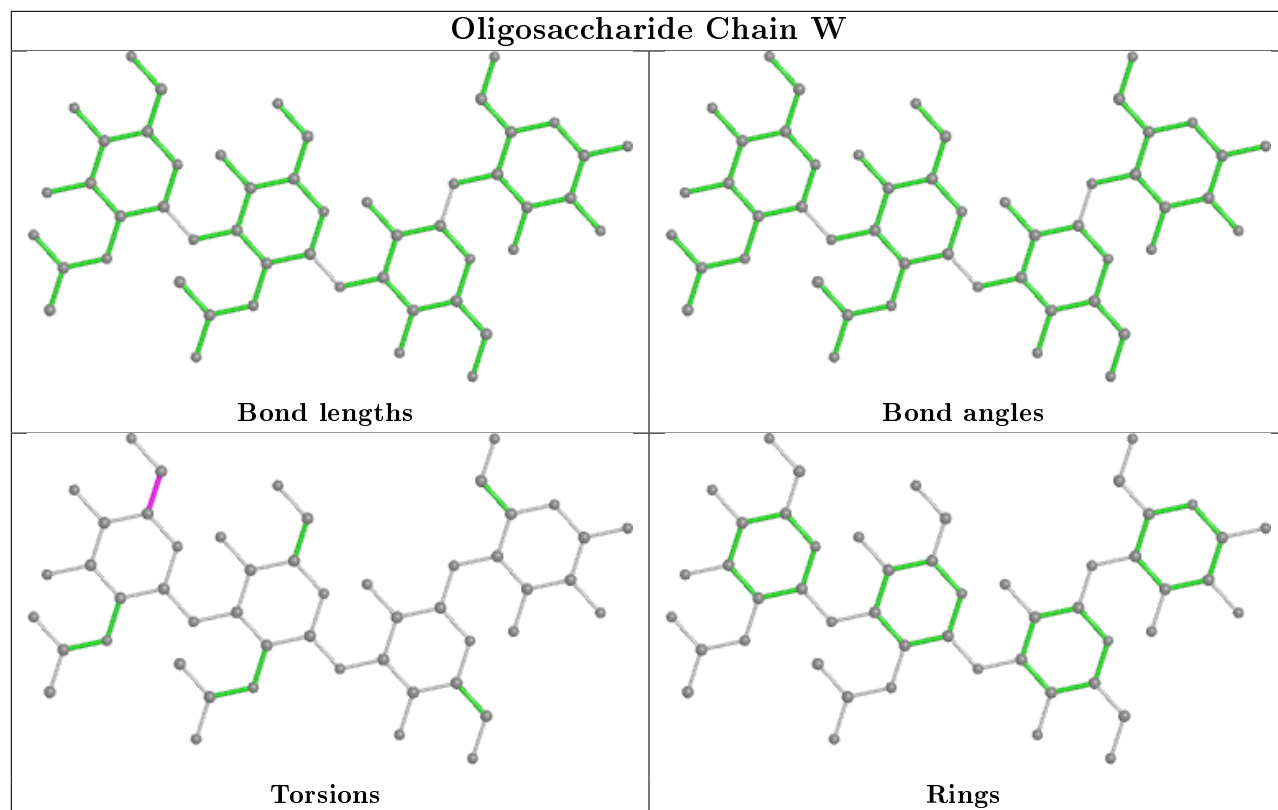












## 5.6 Ligand geometry

1 ligand is 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	GLA	A	107	-	12,12,12	0.44	0	17,17,17	1.05	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
4	GLA	A	107	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	107	GLA	C4-C5-C6-O6
4	A	107	GLA	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	107	GLA	12	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 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	94/94 (100%)	-0.02	0 100 100	31, 62, 91, 103	0
1	B	94/94 (100%)	0.08	0 100 100	36, 61, 85, 101	0
1	C	94/94 (100%)	0.00	0 100 100	36, 64, 88, 106	0
1	D	94/94 (100%)	0.23	0 100 100	35, 70, 95, 108	0
1	E	94/94 (100%)	0.11	1 (1%) 80 79	35, 72, 101, 117	0
1	F	94/94 (100%)	0.15	1 (1%) 80 79	39, 67, 93, 118	0
1	G	94/94 (100%)	0.34	2 (2%) 63 62	52, 90, 123, 144	0
1	H	94/94 (100%)	0.33	1 (1%) 80 79	45, 79, 125, 148	0
1	I	94/94 (100%)	0.18	0 100 100	38, 74, 120, 135	0
1	J	94/94 (100%)	0.67	9 (9%) 8 9	90, 130, 165, 192	0
1	K	94/94 (100%)	1.09	17 (18%) 1 1	102, 142, 171, 197	0
1	L	94/94 (100%)	1.55	32 (34%) 0 0	94, 133, 167, 175	0
All	All	1128/1128 (100%)	0.39	63 (5%) 24 25	31, 78, 154, 197	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	61	SER	5.7
1	J	4	HIS	5.7
1	K	62	SER	5.4
1	K	63	ALA	4.5
1	L	78	TRP	4.2
1	G	94	ASP	4.0
1	L	64	ASP	3.7
1	L	66	VAL	3.7
1	J	88	LEU	3.4
1	J	78	TRP	3.4
1	L	21	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	59	VAL	3.3
1	K	59	VAL	3.3
1	L	15	HIS	3.2
1	L	71	PHE	3.2
1	L	83	VAL	3.2
1	L	24	THR	3.2
1	J	77	SER	3.2
1	L	13	SER	3.1
1	K	18	TRP	3.0
1	K	33	TRP	2.9
1	L	51	VAL	2.9
1	L	63	ALA	2.9
1	K	40	PRO	2.8
1	K	64	ASP	2.8
1	K	50	ASP	2.8
1	L	77	SER	2.8
1	E	78	TRP	2.7
1	L	86	TYR	2.7
1	G	2	LEU	2.7
1	K	94	ASP	2.7
1	L	29	PRO	2.7
1	L	27	ASP	2.6
1	L	48	MET	2.6
1	K	75	TYR	2.5
1	L	42	VAL	2.5
1	J	5	VAL	2.5
1	K	42	VAL	2.5
1	L	33	TRP	2.5
1	L	82	THR	2.5
1	L	62	SER	2.5
1	K	66	VAL	2.5
1	F	57	LEU	2.5
1	L	94	ASP	2.4
1	J	16	ARG	2.4
1	L	52	ASP	2.3
1	L	74	HIS	2.3
1	L	72	THR	2.3
1	L	26	SER	2.3
1	L	49	LEU	2.3
1	L	79	TYR	2.3
1	J	82	THR	2.3
1	L	65	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	19	PRO	2.2
1	K	67	THR	2.2
1	K	85	ASN	2.2
1	J	84	TRP	2.2
1	J	13	SER	2.2
1	L	85	ASN	2.1
1	K	15	HIS	2.1
1	L	57	LEU	2.0
1	H	32	PHE	2.0
1	L	17	CYS	2.0

## 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
2	NAG	c	2	14/15	0.67	0.57	152,152,152,152	0
3	GAL	d	1	12/12	0.67	0.40	164,164,164,164	0
2	NAG	e	2	14/15	0.72	0.62	152,152,152,152	0
3	NGA	d	3	14/15	0.73	0.42	155,155,155,155	0
3	A2G	a	4	14/15	0.74	0.34	118,118,118,118	0
3	GLA	d	2	11/12	0.74	0.27	168,168,168,168	0
2	NAG	e	1	14/15	0.76	0.34	147,147,147,147	0
2	NAG	V	2	14/15	0.76	0.29	117,117,117,117	0
3	GAL	f	1	12/12	0.78	0.54	166,166,166,166	0
3	GAL	Y	1	12/12	0.79	0.32	116,116,116,116	0
3	A2G	d	4	14/15	0.79	0.28	138,138,138,138	0
3	NGA	f	3	14/15	0.80	0.38	176,176,176,176	0
2	NAG	M	2	14/15	0.80	0.43	115,115,115,115	0
2	NAG	g	2	14/15	0.80	0.33	133,133,133,133	0
3	GAL	N	1	12/12	0.80	0.41	111,111,111,111	0
2	NAG	b	2	14/15	0.81	0.43	154,154,154,154	0
3	GAL	S	1	12/12	0.82	0.29	87,87,87,87	0
2	NAG	c	1	14/15	0.82	0.38	146,146,146,146	0

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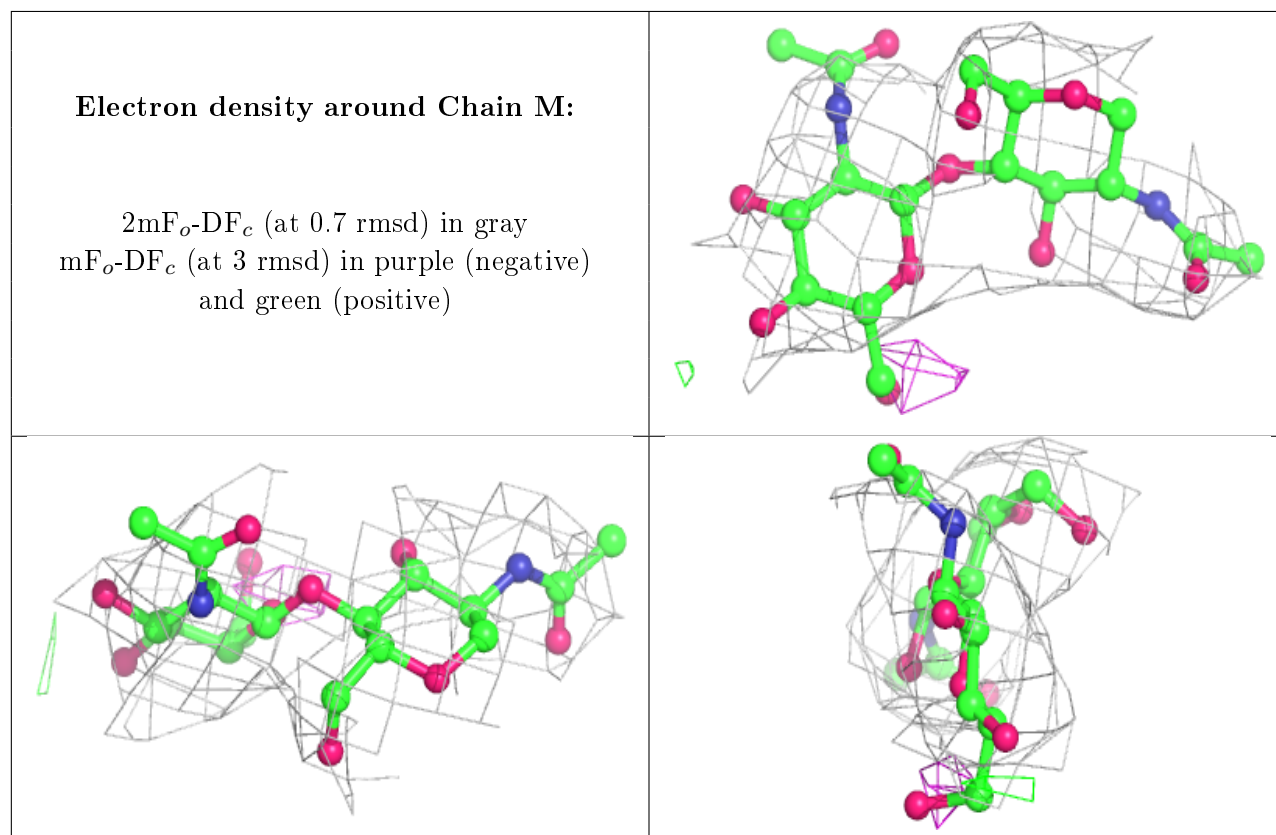
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	Q	2	14/15	0.82	0.37	129,129,129,129	0
2	NAG	X	2	14/15	0.83	0.28	126,126,126,126	0
2	NAG	O	2	14/15	0.83	0.30	116,116,116,116	0
3	GLA	f	2	11/12	0.84	0.37	186,186,186,186	0
3	A2G	Y	4	14/15	0.84	0.26	81,81,81,81	0
3	GAL	h	1	12/12	0.84	0.32	123,123,123,123	0
2	NAG	R	2	14/15	0.85	0.30	114,114,114,114	0
3	GLA	Y	2	11/12	0.85	0.25	118,118,118,118	0
3	A2G	h	4	14/15	0.85	0.51	146,146,146,146	0
3	A2G	f	4	14/15	0.86	0.20	143,143,143,143	0
3	NGA	h	3	14/15	0.86	0.44	136,136,136,136	0
3	GAL	W	1	12/12	0.86	0.24	96,96,96,96	0
3	GLA	h	2	11/12	0.86	0.28	131,131,131,131	0
3	NGA	a	3	14/15	0.87	0.27	105,105,105,105	0
3	GLA	N	2	11/12	0.87	0.33	97,97,97,97	0
2	NAG	g	1	14/15	0.87	0.42	121,121,121,121	0
3	GAL	P	1	12/12	0.87	0.21	99,99,99,99	0
2	NAG	T	2	14/15	0.87	0.47	144,144,144,144	0
2	NAG	X	1	14/15	0.88	0.21	73,73,73,73	0
3	GAL	U	1	12/12	0.88	0.24	101,101,101,101	0
2	NAG	R	1	14/15	0.89	0.33	79,79,79,79	0
3	A2G	W	4	14/15	0.89	0.25	64,64,64,64	0
3	NGA	U	3	14/15	0.89	0.24	92,92,92,92	0
3	NGA	W	3	14/15	0.89	0.21	84,84,84,84	0
3	NGA	N	3	14/15	0.90	0.24	73,73,73,73	0
3	NGA	Y	3	14/15	0.90	0.26	83,83,83,83	0
3	GLA	S	2	11/12	0.90	0.16	98,98,98,98	0
3	NGA	P	3	14/15	0.90	0.19	86,86,86,86	0
3	NGA	S	3	14/15	0.90	0.20	117,117,117,117	0
2	NAG	V	1	14/15	0.91	0.24	72,72,72,72	0
3	A2G	U	4	14/15	0.91	0.27	76,76,76,76	0
3	GLA	P	2	11/12	0.91	0.14	101,101,101,101	0
2	NAG	Z	2	14/15	0.91	0.17	79,79,79,79	0
3	GAL	a	1	12/12	0.92	0.25	68,68,68,68	0
3	GLA	U	2	11/12	0.92	0.22	102,102,102,102	0
2	NAG	T	1	14/15	0.93	0.28	76,76,76,76	0
2	NAG	Z	1	14/15	0.93	0.21	79,79,79,79	0
2	NAG	Q	1	14/15	0.93	0.26	68,68,68,68	0
2	NAG	M	1	14/15	0.93	0.23	64,64,64,64	0
3	A2G	S	4	14/15	0.93	0.21	77,77,77,77	0
2	NAG	b	1	14/15	0.93	0.22	89,89,89,89	0
3	GLA	W	2	11/12	0.94	0.13	106,106,106,106	0

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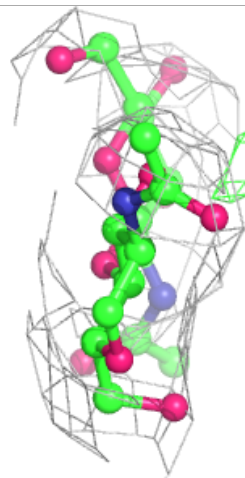
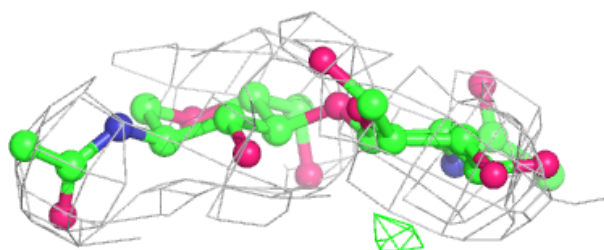
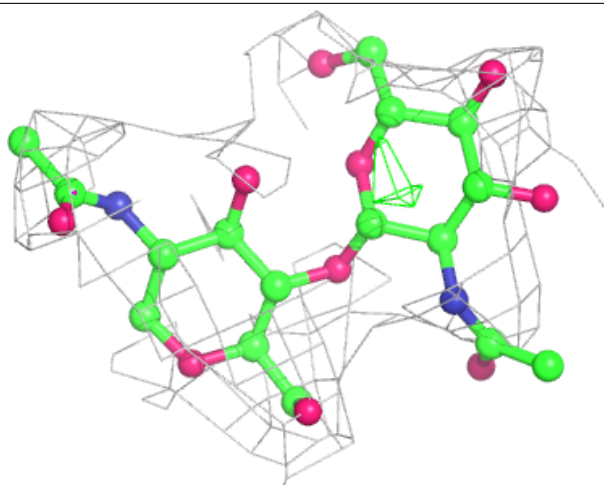
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A2G	N	4	14/15	0.95	0.24	52,52,52,52	0
2	NAG	O	1	14/15	0.95	0.21	67,67,67,67	0
3	A2G	P	4	14/15	0.96	0.23	67,67,67,67	0
3	GLA	a	2	11/12	0.97	0.19	59,59,59,59	0

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.



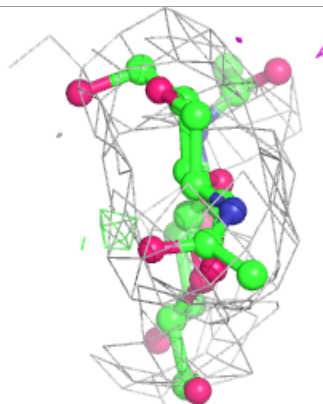
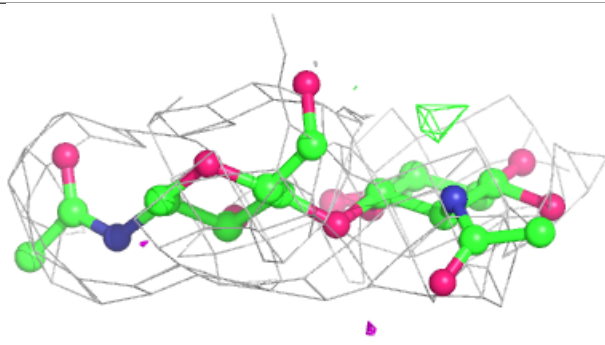
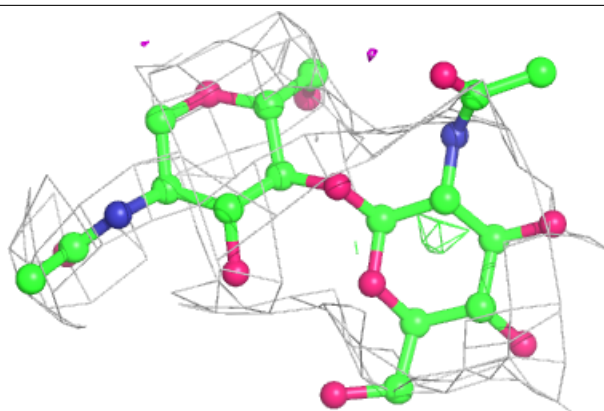
**Electron density around Chain O:**

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

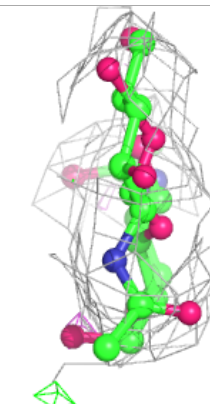
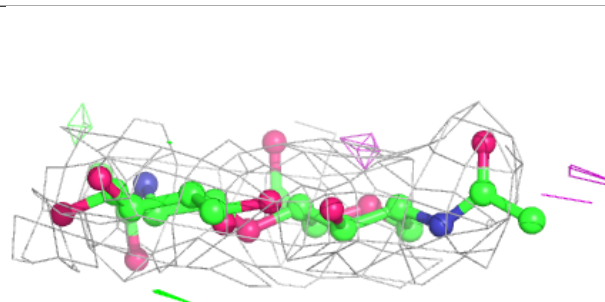
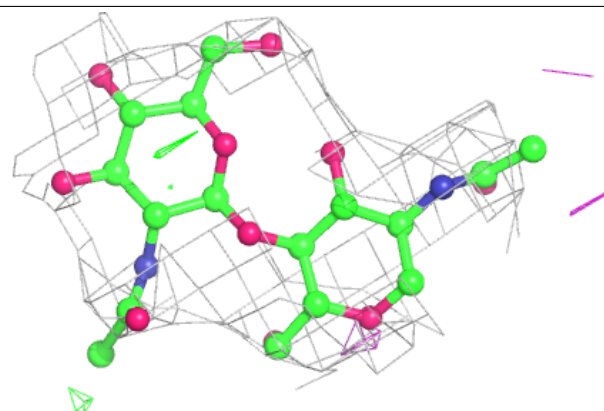


**Electron density around Chain Q:**

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

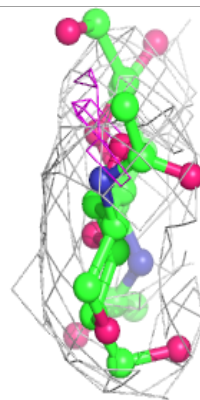
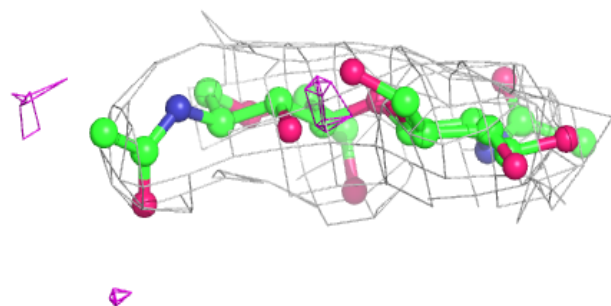
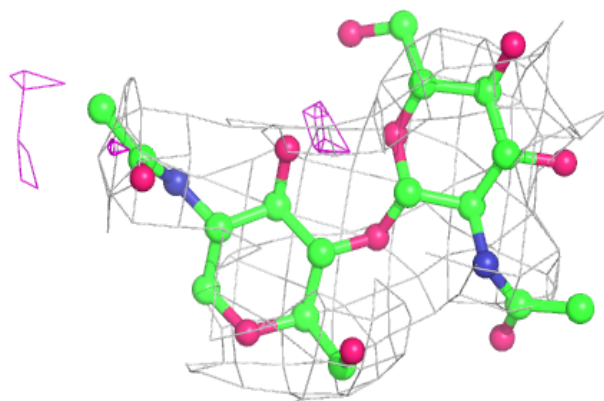
**Electron density around Chain R:**

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



**Electron density around Chain T:**

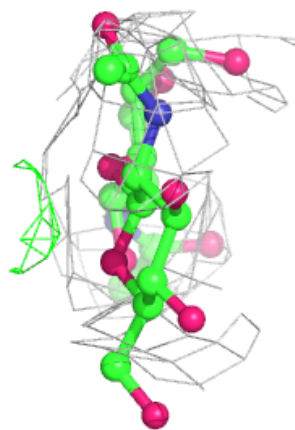
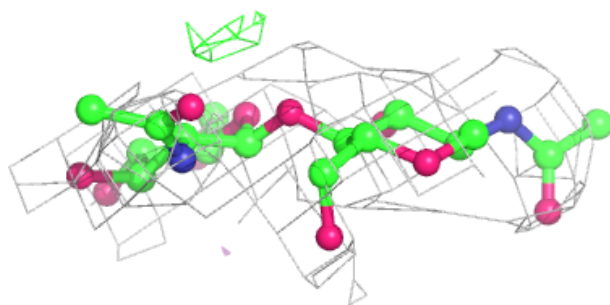
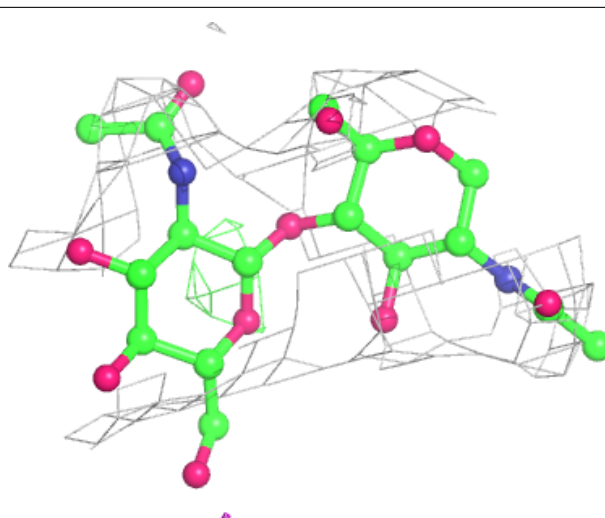
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





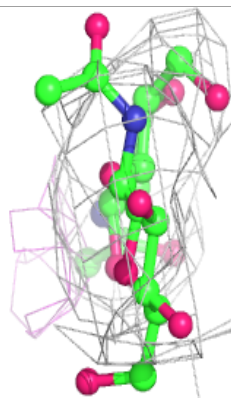
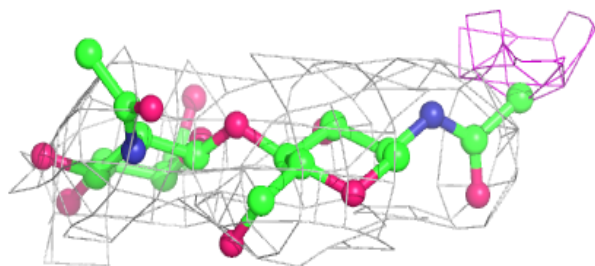
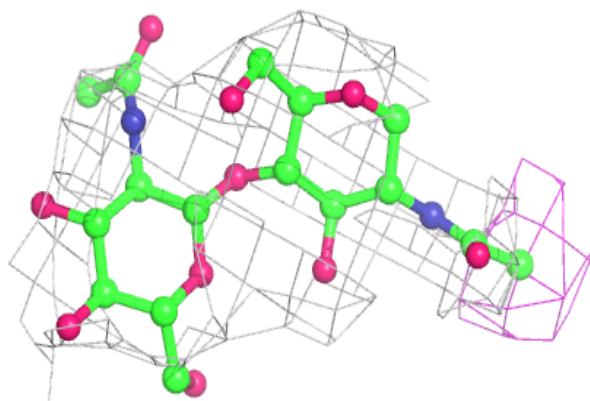
**Electron density around Chain V:**

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

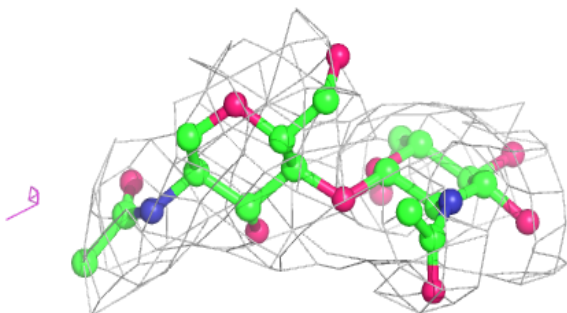
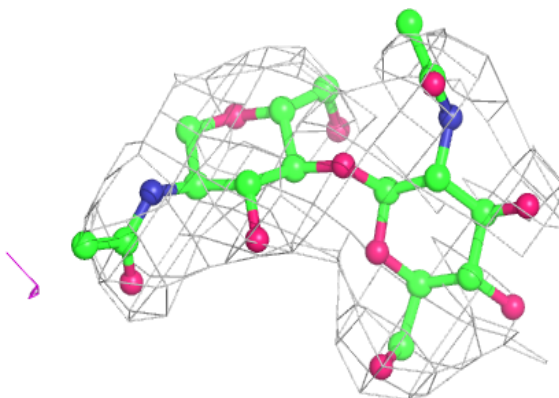


**Electron density around Chain X:**

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

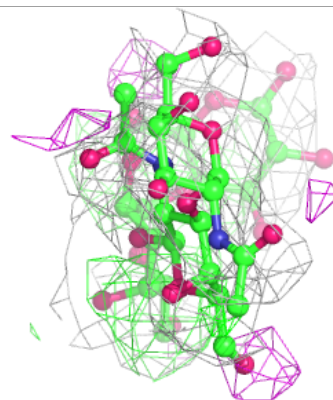
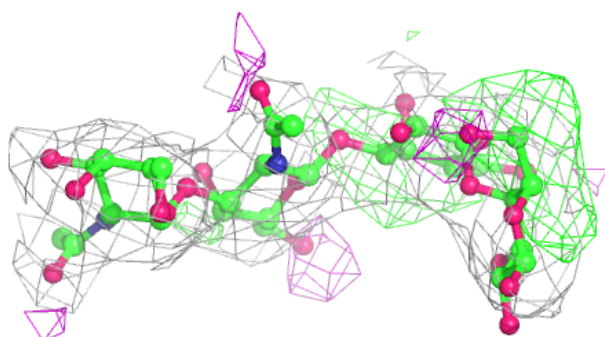
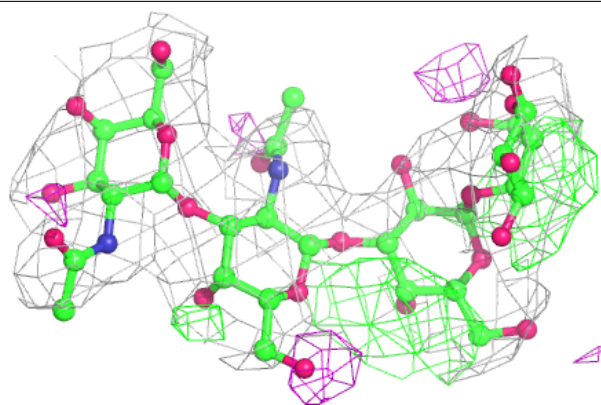
**Electron density around Chain Z:**

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

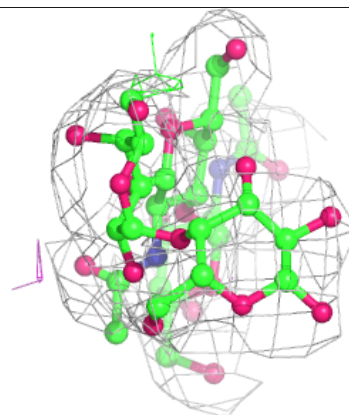
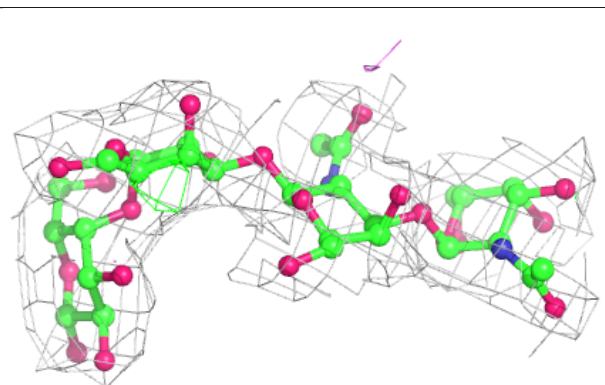
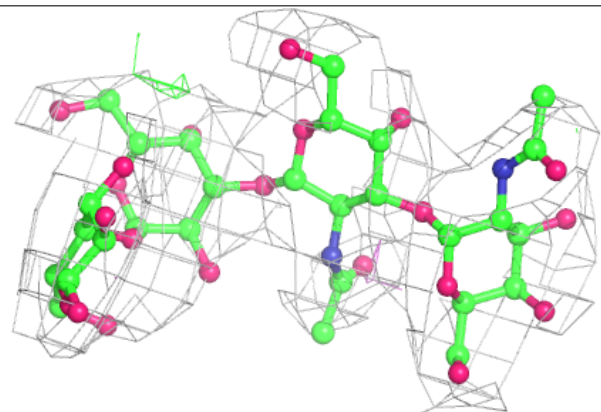


**Electron density around Chain N:**

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

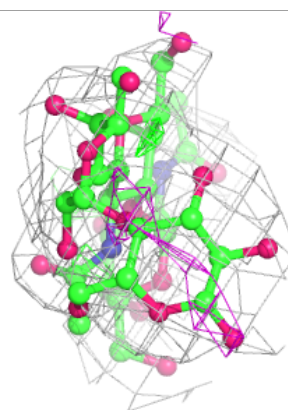
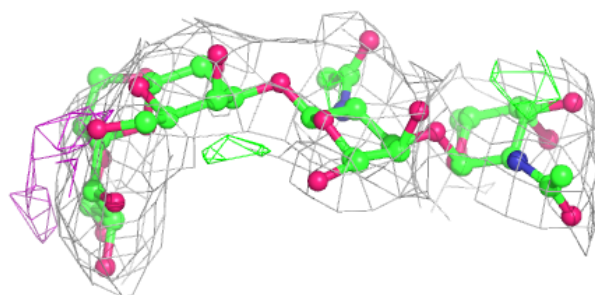
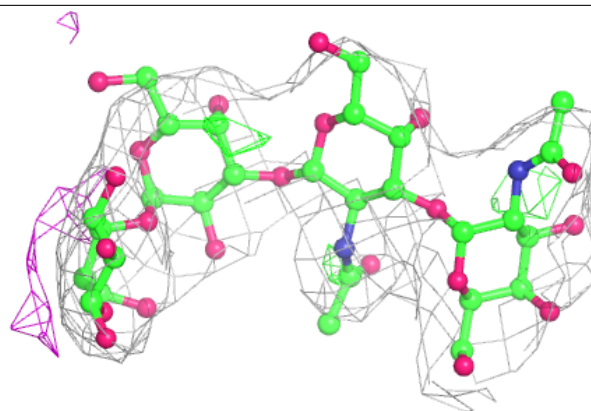
**Electron density around Chain P:**

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

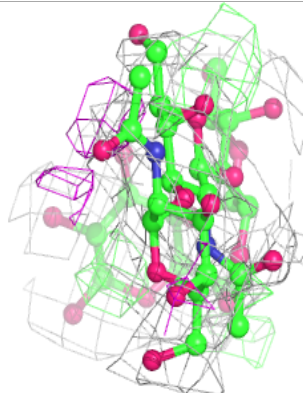
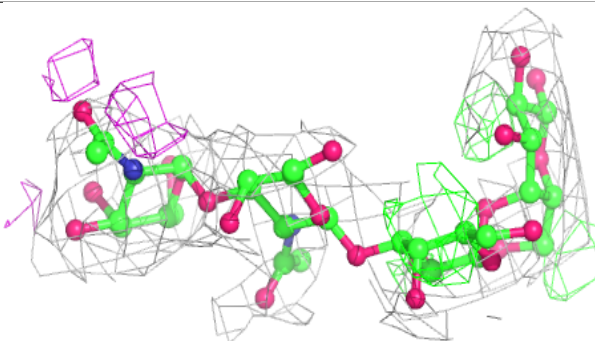
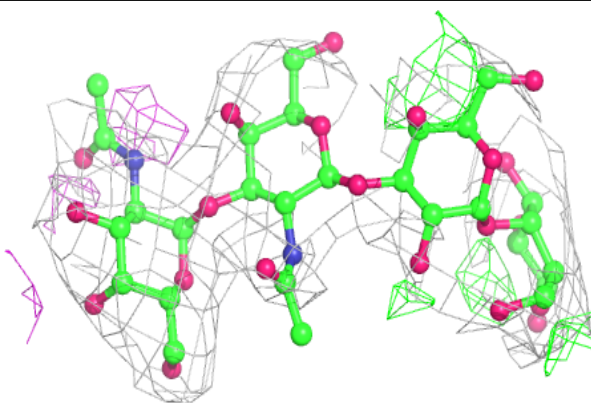


**Electron density around Chain S:**

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

**Electron density around Chain U:**

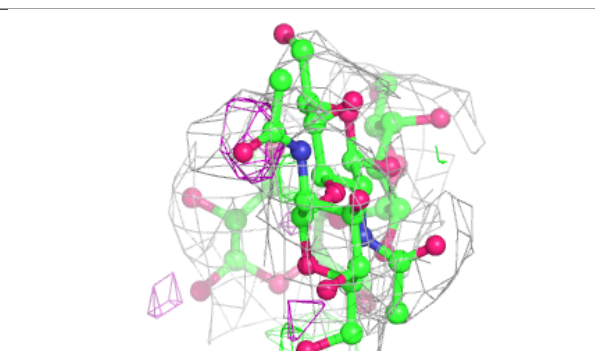
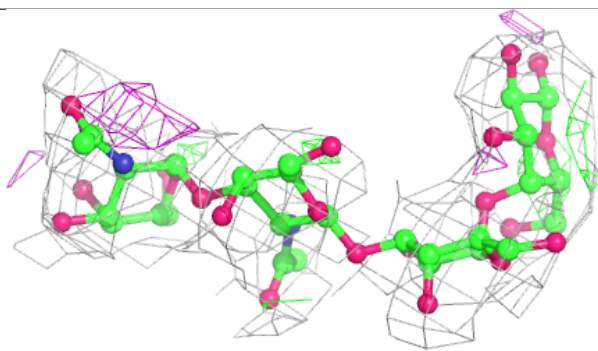
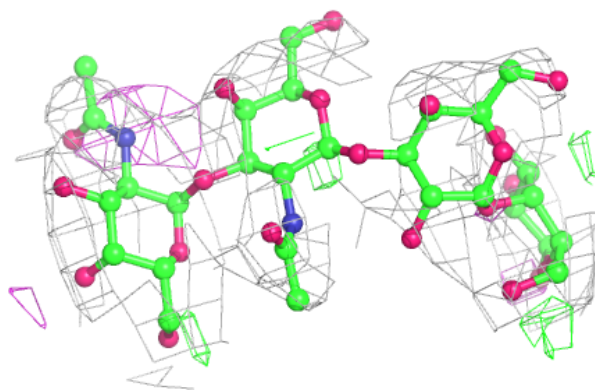
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



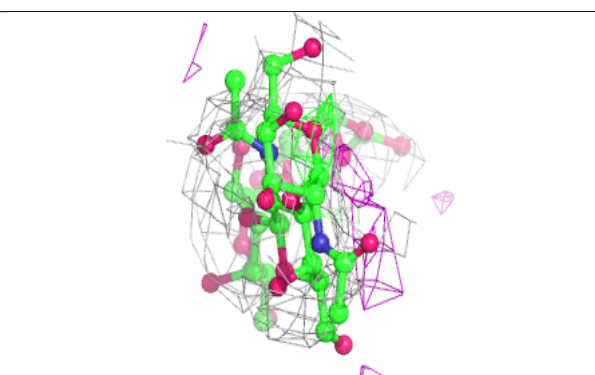
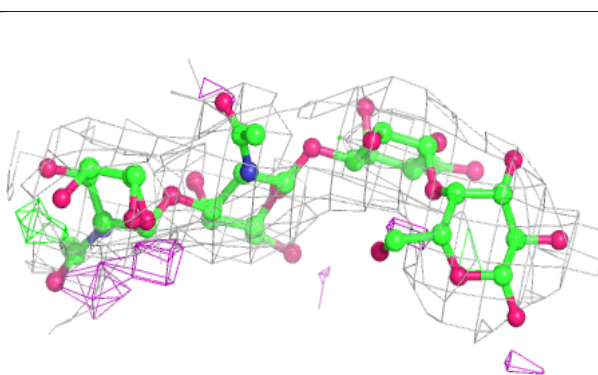
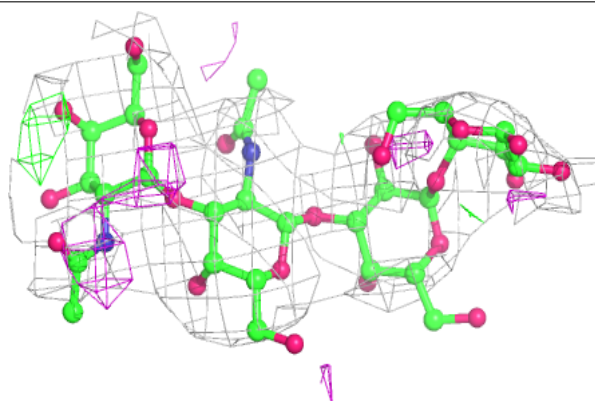


**Electron density around Chain W:**

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

**Electron density around Chain Y:**

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



## 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GLA	A	107	12/12	0.84	0.38	135,135,135,135	0

## 6.5 Other polymers

There are no such residues in this entry.