



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:31 PM BST

PDB ID : 1M26  
Title : Crystal structure of jacalin-T-antigen complex  
Authors : Jeyapakash, A.A.; Rani, P.G.; Reddy, G.B.; Banumathi, S.; Betzel, C.; Suro-  
lia, A.; Vijayan, M.  
Deposited on : 2002-06-21  
Resolution : 1.62 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

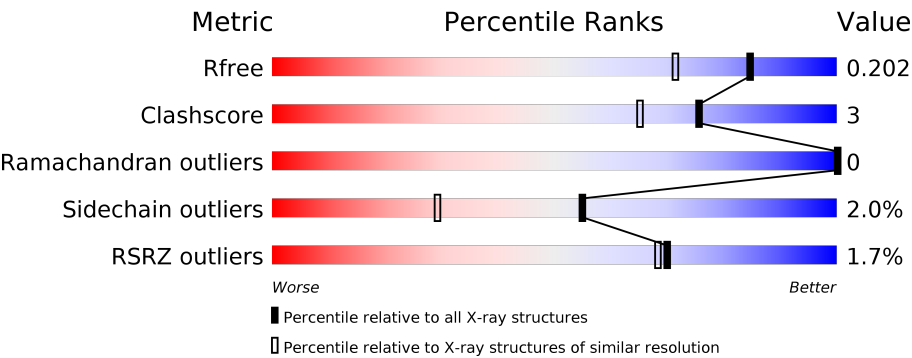
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.62 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.





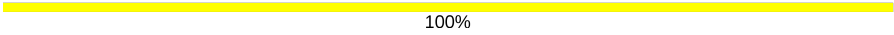
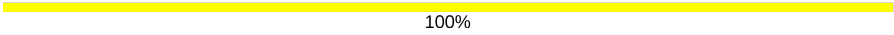
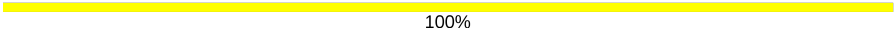
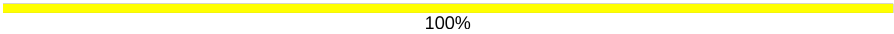
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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	133	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>90%9%</div></div>
1	C	133	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>92%7%</div></div>
1	E	133	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>88%10%</div></div>
1	G	133	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>94%5%</div></div>
2	B	17	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>6%59%24%6%12%</div></div>
2	D	17	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>12%94%6%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	17	
2	H	17	
3	I	2	
3	J	2	
3	K	2	
3	L	2	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5187 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 Jacalin, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1036	676	159	199	2			
1	C	133	Total	C	N	O	S	0	0	0
			1040	679	160	199	2			
1	E	133	Total	C	N	O	S	0	0	0
			1040	679	160	199	2			
1	G	133	Total	C	N	O	S	0	0	0
			1036	676	159	199	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	VAL	ILE	conflict	GB 289162
C	98	VAL	ILE	conflict	GB 289162
E	98	VAL	ILE	conflict	GB 289162
G	98	VAL	ILE	conflict	GB 289162

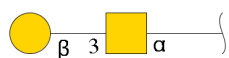
- Molecule 2 is a protein called Jacalin, beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	0	0	0
			105	68	18	19			
2	D	17	Total	C	N	O	0	0	0
			117	74	20	23			
2	F	15	Total	C	N	O	0	0	0
			105	68	18	19			
2	H	15	Total	C	N	O	0	0	0
			105	68	18	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	SER	VAL	conflict	GB 289162
B	20	ALA	SER	conflict	GB 289162
D	19	SER	VAL	conflict	GB 289162
D	20	ALA	SER	conflict	GB 289162
F	19	SER	VAL	conflict	GB 289162
F	20	ALA	SER	conflict	GB 289162
H	19	SER	VAL	conflict	GB 289162
H	20	ALA	SER	conflict	GB 289162

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	N	O	0	0	0
			26	14	1	11			
3	J	2	Total	C	N	O	0	1	0
			27	14	1	12			
3	K	2	Total	C	N	O	0	1	0
			27	14	1	12			
3	L	2	Total	C	N	O	0	0	0
			26	14	1	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total	O	0	0
			141	141		
4	B	15	Total	O	0	0
			15	15		
4	C	105	Total	O	0	0
			105	105		
4	D	19	Total	O	0	0
			19	19		
4	E	97	Total	O	0	0
			97	97		
4	F	16	Total	O	0	0
			16	16		
4	G	92	Total	O	0	0
			92	92		

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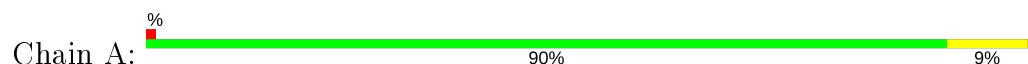
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	12	Total	O	0	0
			12	12		

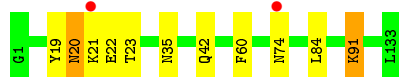
### 3 Residue-property plots [i](#)

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.

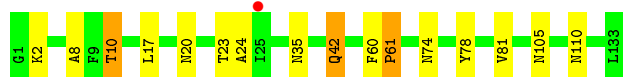
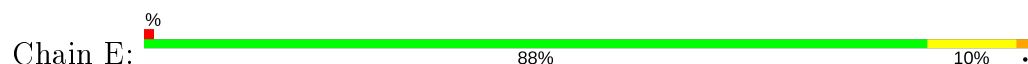
- Molecule 1: Jacalin, alpha chain



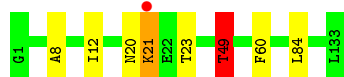
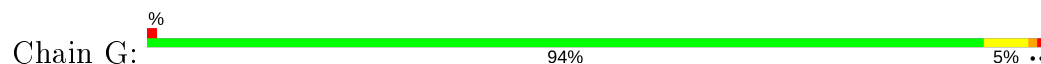
- Molecule 1: Jacalin, alpha chain



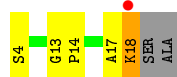
- Molecule 1: Jacalin, alpha chain



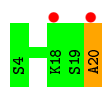
- Molecule 1: Jacalin, alpha chain



- Molecule 2: Jacalin, beta chain



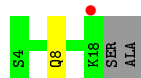
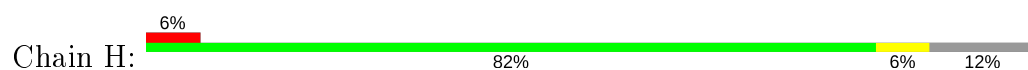
- Molecule 2: Jacalin, beta chain



- Molecule 2: Jacalin, beta chain



- Molecule 2: Jacalin, beta chain



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



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



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.92Å 78.00Å 67.91Å 90.00° 100.73° 90.00°	Depositor
Resolution (Å)	19.58 – 1.62 19.58 – 1.62	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.58-1.62) 96.8 (19.58-1.62)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.62Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.189 , 0.206 0.185 , 0.202	Depositor DCC
$R_{free}$ test set	3787 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, 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	0.43	0/1065	0.88	6/1445 (0.4%)
1	C	0.39	0/1069	1.07	5/1449 (0.3%)
1	E	0.54	2/1069 (0.2%)	1.00	7/1449 (0.5%)
1	G	0.38	0/1065	0.80	6/1445 (0.4%)
2	B	0.76	0/107	1.71	2/145 (1.4%)
2	D	0.57	0/119	1.23	1/160 (0.6%)
2	F	0.83	0/107	1.81	4/145 (2.8%)
2	H	0.78	0/107	1.13	0/145
All	All	0.48	2/4708 (0.0%)	1.01	31/6383 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	61	PRO	C-N	8.92	1.54	1.34
1	E	61	PRO	N-CD	-5.33	1.40	1.47

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	LYS	CA-CB-CG	26.04	170.68	113.40
1	E	60	PHE	C-N-CD	-12.86	92.30	120.60
2	B	17	ALA	CB-CA-C	-10.47	94.40	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	9	THR	N-CA-CB	-10.16	91.00	110.30
1	E	60	PHE	C-N-CA	10.03	164.12	122.00
1	E	61	PRO	N-CD-CG	9.70	117.75	103.20
2	F	8	GLN	CB-CA-C	9.68	129.75	110.40
1	E	61	PRO	O-C-N	-9.56	107.40	122.70
1	C	60	PHE	C-N-CD	-9.43	99.85	120.60
2	D	20	ALA	N-CA-C	8.87	134.94	111.00
1	C	91	LYS	CG-CD-CE	8.84	138.41	111.90
1	A	60	PHE	C-N-CD	-8.56	101.77	120.60
2	F	18	LYS	N-CA-C	-7.98	89.46	111.00
1	E	61	PRO	CA-N-CD	-7.84	100.52	111.50
1	A	42	GLN	CB-CA-C	7.38	125.15	110.40
1	E	42	GLN	CA-CB-CG	6.89	128.56	113.40
2	B	18	LYS	N-CA-C	6.52	128.61	111.00
1	G	12	ILE	CG1-CB-CG2	6.44	125.57	111.40
1	A	45	LYS	CB-CA-C	-6.20	98.00	110.40
1	G	49	THR	N-CA-CB	-6.17	98.58	110.30
1	G	12	ILE	CA-CB-CG1	-5.97	99.65	111.00
2	F	18	LYS	CB-CA-C	5.95	122.30	110.40
1	A	60	PHE	C-N-CA	5.91	146.83	122.00
1	G	60	PHE	C-N-CD	-5.78	107.88	120.60
1	G	84	LEU	CA-CB-CG	5.51	127.96	115.30
1	A	60	PHE	O-C-N	-5.50	110.66	121.10
1	C	74	ASN	N-CA-CB	-5.40	100.88	110.60
1	E	10	THR	N-CA-CB	5.38	120.52	110.30
1	C	60	PHE	C-N-CA	5.26	144.11	122.00
1	G	60	PHE	C-N-CA	5.07	143.31	122.00
1	A	91	LYS	CA-CB-CG	5.02	124.45	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	61	PRO	Mainchain

## 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	1036	0	998	7	0
1	C	1040	0	1009	8	0
1	E	1040	0	1009	9	0
1	G	1036	0	998	5	0
2	B	105	0	108	3	0
2	D	117	0	118	1	0
2	F	105	0	108	0	0
2	H	105	0	108	1	0
3	I	26	0	21	0	0
3	J	27	0	10	0	0
3	K	27	0	10	0	0
3	L	26	0	21	0	0
4	A	141	0	0	2	0
4	B	15	0	0	2	0
4	C	105	0	0	1	0
4	D	19	0	0	1	0
4	E	97	0	0	2	0
4	F	16	0	0	0	0
4	G	92	0	0	1	0
4	H	12	0	0	0	0
All	All	5187	0	4518	29	0

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

All (29) 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:G:49:THR:OG1	4:G:621:HOH:O	1.78	1.00
1:C:20:ASN:HD22	1:C:22:GLU:H	1.36	0.74
1:E:42:GLN:NE2	4:E:518:HOH:O	2.25	0.70
2:B:4:SER:HB3	4:B:685:HOH:O	2.00	0.61
1:E:110:ASN:HD21	2:H:8:GLN:HE21	1.47	0.61
2:D:20:ALA:HB3	4:D:373:HOH:O	2.05	0.56
1:A:21:LYS:HG2	4:A:229:HOH:O	2.07	0.54
1:A:19:TYR:HE1	1:A:54:VAL:CG2	2.21	0.54
2:B:18:LYS:NZ	4:B:657:HOH:O	2.40	0.53
1:A:19:TYR:HE1	1:A:54:VAL:HG23	1.75	0.51
1:E:20:ASN:HB3	1:E:23:THR:OG1	2.11	0.51
1:C:20:ASN:ND2	1:C:22:GLU:H	2.06	0.51
1:C:20:ASN:C	1:C:20:ASN:HD22	2.15	0.50
1:C:20:ASN:HB3	1:C:23:THR:OG1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:LYS:HB3	1:G:21:LYS:NZ	2.29	0.48
1:C:35:ASN:HD21	1:G:8:ALA:H	1.62	0.47
1:E:74:ASN:HA	1:E:78:TYR:O	2.16	0.45
1:C:35:ASN:ND2	1:G:8:ALA:H	2.14	0.45
1:C:19:TYR:HE2	1:C:21:LYS:HG3	1.82	0.44
1:A:87:LYS:HE2	4:A:418:HOH:O	2.17	0.44
1:C:42:GLN:NE2	4:C:422:HOH:O	2.50	0.44
1:A:8:ALA:H	1:E:35:ASN:HD21	1.67	0.42
2:B:13:GLY:HA3	2:B:14:PRO:HA	1.73	0.42
1:E:2:LYS:HE3	4:E:242:HOH:O	2.20	0.41
1:E:17:LEU:HD12	1:E:17:LEU:C	2.40	0.41
1:A:105:ASN:HD22	1:A:105:ASN:N	2.18	0.41
1:E:24:ALA:HB1	1:E:81:VAL:O	2.20	0.41
1:G:20:ASN:HB3	1:G:23:THR:OG1	2.21	0.41
1:A:35:ASN:HD21	1:E:8:ALA:H	1.69	0.41

There are no symmetry-related clashes.

## 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	131/133 (98%)	128 (98%)	3 (2%)	0	100	100
1	C	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
1	E	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
1	G	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
2	B	13/17 (76%)	13 (100%)	0	0	100	100
2	D	15/17 (88%)	15 (100%)	0	0	100	100
2	F	13/17 (76%)	13 (100%)	0	0	100	100
2	H	13/17 (76%)	13 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	578/600 (96%)	559 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/113 (99%)	109 (97%)	3 (3%)	44	18
1	C	113/113 (100%)	110 (97%)	3 (3%)	44	18
1	E	113/113 (100%)	111 (98%)	2 (2%)	59	34
1	G	112/113 (99%)	110 (98%)	2 (2%)	59	34
2	B	11/12 (92%)	11 (100%)	0	100	100
2	D	12/12 (100%)	12 (100%)	0	100	100
2	F	11/12 (92%)	11 (100%)	0	100	100
2	H	11/12 (92%)	11 (100%)	0	100	100
All	All	495/500 (99%)	485 (98%)	10 (2%)	55	29

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LEU
1	A	105	ASN
1	A	107	PRO
1	C	20	ASN
1	C	84	LEU
1	C	91	LYS
1	E	10	THR
1	E	105	ASN
1	G	21	LYS
1	G	49	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	105	ASN
1	C	20	ASN
1	C	35	ASN
1	C	42	GLN
1	C	110	ASN
2	D	8	GLN
1	E	29	GLN
1	E	35	ASN
1	E	105	ASN
2	F	8	GLN
1	G	35	ASN
1	G	110	ASN
2	H	8	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

10 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	A2G	I	1	3	15,15,15	1.59	4 (26%)	21,21,21	2.30	4 (19%)
3	GAL	I	2	3	11,11,12	1.89	3 (27%)	15,15,17	2.90	4 (26%)
3	A2G	J	1[A]	-	15,15,15	1.83	4 (26%)	21,21,21	1.63	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	A2G	J	1[B]	-	15,15,15	1.85	4 (26%)	21,21,21	2.70	4 (19%)
3	GAL	J	2	3	11,11,12	1.55	3 (27%)	15,15,17	3.03	4 (26%)
3	A2G	K	1[A]	-	15,15,15	1.75	4 (26%)	21,21,21	1.53	3 (14%)
3	A2G	K	1[B]	-	15,15,15	1.71	4 (26%)	21,21,21	1.43	2 (9%)
3	GAL	K	2	3	11,11,12	1.82	4 (36%)	15,15,17	3.07	4 (26%)
3	A2G	L	1	3	15,15,15	1.68	4 (26%)	21,21,21	1.47	2 (9%)
3	GAL	L	2	3	11,11,12	1.86	4 (36%)	15,15,17	3.26	6 (40%)

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	A2G	I	1	3	-	0/6/26/26	0/1/1/1
3	GAL	I	2	3	-	0/2/19/22	0/1/1/1
3	A2G	J	1[A]	-	-	0/6/26/26	0/1/1/1
3	A2G	J	1[B]	-	-	0/6/26/26	0/1/1/1
3	GAL	J	2	3	-	0/2/19/22	0/1/1/1
3	A2G	K	1[A]	-	-	2/6/26/26	0/1/1/1
3	A2G	K	1[B]	-	-	2/6/26/26	0/1/1/1
3	GAL	K	2	3	-	0/2/19/22	0/1/1/1
3	A2G	L	1	3	-	1/6/26/26	0/1/1/1
3	GAL	L	2	3	-	0/2/19/22	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	2	GAL	O5-C5	4.07	1.51	1.43
3	L	2	GAL	O5-C5	3.98	1.51	1.43
3	K	2	GAL	O5-C5	3.76	1.51	1.43
3	J	1[B]	A2G	C2-N2	-3.67	1.40	1.45
3	J	1[A]	A2G	C2-N2	-3.67	1.40	1.45
3	K	1[B]	A2G	O5-C5	3.62	1.53	1.44
3	K	1[A]	A2G	O5-C5	3.62	1.53	1.44
3	I	2	GAL	O5-C1	3.41	1.49	1.43
3	J	1[B]	A2G	O5-C5	3.26	1.52	1.44
3	J	1[A]	A2G	O5-C5	3.26	1.52	1.44
3	I	1	A2G	C2-N2	-3.25	1.40	1.45
3	L	1	A2G	O5-C1	3.12	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1[B]	A2G	C4-C5	3.07	1.59	1.53
3	J	1[A]	A2G	C4-C5	3.07	1.59	1.53
3	K	1[B]	A2G	O5-C1	3.06	1.50	1.42
3	K	1[A]	A2G	O5-C1	3.06	1.50	1.42
3	L	1	A2G	O5-C5	3.04	1.51	1.44
3	L	2	GAL	C4-C3	3.01	1.60	1.52
3	K	2	GAL	O5-C1	2.98	1.48	1.43
3	I	1	A2G	O5-C5	2.86	1.51	1.44
3	L	2	GAL	O5-C1	2.84	1.48	1.43
3	J	2	GAL	O5-C5	2.82	1.49	1.43
3	K	1[B]	A2G	C2-N2	-2.81	1.41	1.45
3	K	1[A]	A2G	C2-N2	-2.81	1.41	1.45
3	I	2	GAL	C4-C3	2.78	1.59	1.52
3	K	2	GAL	C4-C3	2.77	1.59	1.52
3	J	1[B]	A2G	O5-C1	2.75	1.49	1.42
3	J	1[A]	A2G	O5-C1	2.75	1.49	1.42
3	I	1	A2G	C4-C5	2.71	1.58	1.53
3	L	1	A2G	C2-N2	-2.59	1.41	1.45
3	J	2	GAL	C4-C3	2.59	1.58	1.52
3	K	1[B]	A2G	C4-C5	2.55	1.58	1.53
3	K	1[A]	A2G	C4-C5	2.55	1.58	1.53
3	L	1	A2G	C4-C5	2.49	1.58	1.53
3	I	1	A2G	O5-C1	2.29	1.48	1.42
3	J	2	GAL	O5-C1	2.25	1.47	1.43
3	K	2	GAL	C4-C5	2.17	1.57	1.53
3	L	2	GAL	C4-C5	2.05	1.57	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1[B]	A2G	O1-C1-C2	8.53	126.94	109.22
3	L	2	GAL	C6-C5-C4	8.34	132.54	113.00
3	I	1	A2G	C1-C2-N2	-8.29	101.12	110.73
3	K	2	GAL	C6-C5-C4	7.86	131.41	113.00
3	J	2	GAL	C6-C5-C4	7.61	130.83	113.00
3	I	2	GAL	O6-C6-C5	7.41	136.71	111.29
3	K	2	GAL	O6-C6-C5	7.16	135.87	111.29
3	I	2	GAL	C6-C5-C4	6.90	129.17	113.00
3	J	2	GAL	O6-C6-C5	6.85	134.78	111.29
3	L	2	GAL	O6-C6-C5	6.82	134.68	111.29
3	J	1[B]	A2G	C1-C2-N2	-5.35	104.53	110.73
3	J	1[A]	A2G	C1-C2-N2	-5.35	104.53	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1[B]	A2G	O1-C1-O5	-5.18	94.82	110.38
3	L	1	A2G	C1-C2-N2	-4.50	105.51	110.73
3	K	1[B]	A2G	C1-C2-N2	-4.26	105.80	110.73
3	K	1[A]	A2G	C1-C2-N2	-4.26	105.80	110.73
3	I	1	A2G	C3-C2-N2	4.13	118.42	110.62
3	J	2	GAL	O5-C5-C6	-3.91	101.08	107.20
3	L	2	GAL	O5-C5-C6	-3.87	101.14	107.20
3	K	2	GAL	O5-C5-C6	-3.44	101.82	107.20
3	L	2	GAL	C1-O5-C5	3.31	116.68	112.19
3	J	2	GAL	C1-O5-C5	3.24	116.58	112.19
3	I	2	GAL	C1-O5-C5	3.11	116.41	112.19
3	K	2	GAL	C1-O5-C5	3.05	116.32	112.19
3	L	1	A2G	O5-C5-C6	2.81	113.42	106.44
3	K	1[A]	A2G	O1-C1-C2	2.77	114.97	109.22
3	J	1[B]	A2G	O5-C5-C6	2.76	113.29	106.44
3	J	1[A]	A2G	O5-C5-C6	2.76	113.29	106.44
3	K	1[B]	A2G	O5-C5-C6	2.75	113.27	106.44
3	K	1[A]	A2G	O5-C5-C6	2.75	113.27	106.44
3	L	2	GAL	C3-C4-C5	-2.53	105.72	110.24
3	I	2	GAL	O5-C5-C6	-2.21	103.74	107.20
3	I	1	A2G	C3-C4-C5	-2.20	106.32	110.24
3	I	1	A2G	O5-C5-C6	2.11	111.67	106.44
3	L	2	GAL	C1-C2-C3	2.00	112.13	109.67

There are no chirality outliers.

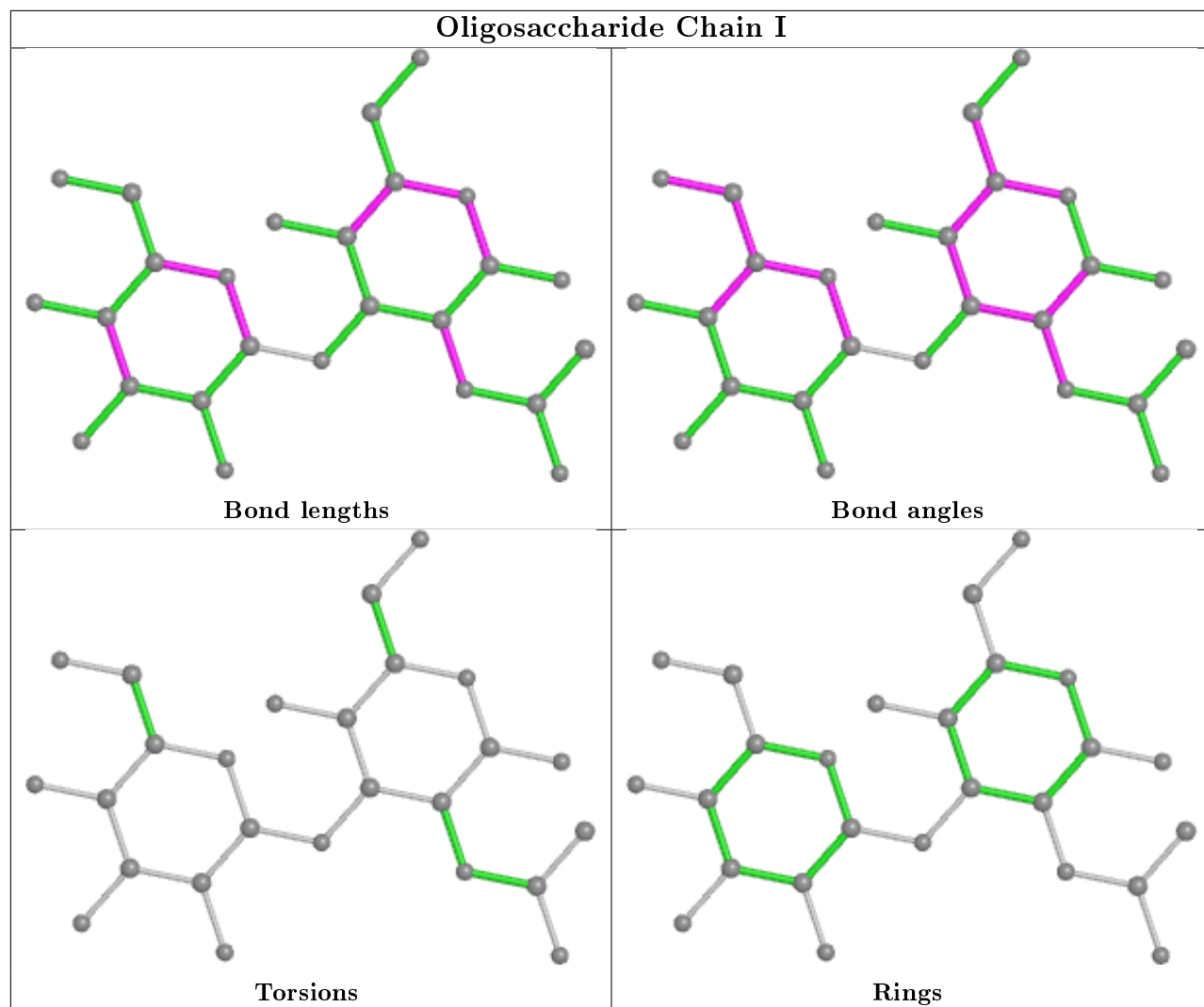
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1[B]	A2G	C4-C5-C6-O6
3	K	1[A]	A2G	C4-C5-C6-O6
3	K	1[B]	A2G	O5-C5-C6-O6
3	K	1[A]	A2G	O5-C5-C6-O6
3	L	1	A2G	C4-C5-C6-O6

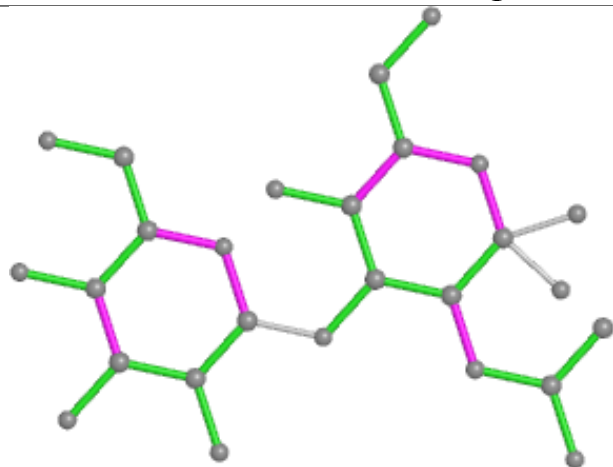
There are no ring outliers.

No monomer is involved in short contacts.

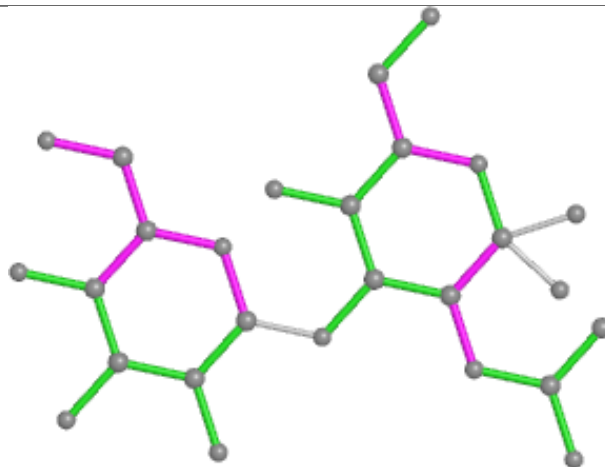
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



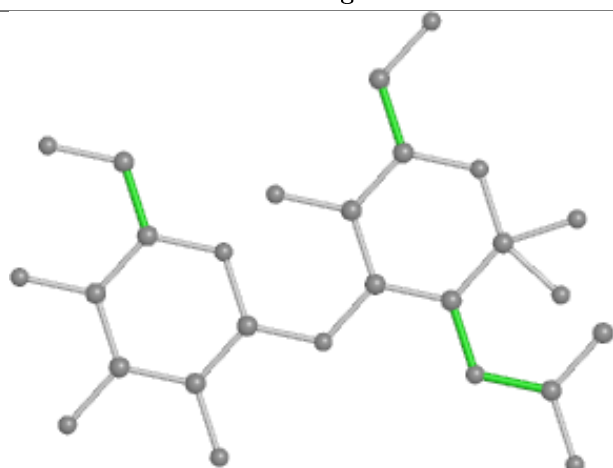
## Oligosaccharide Chain J



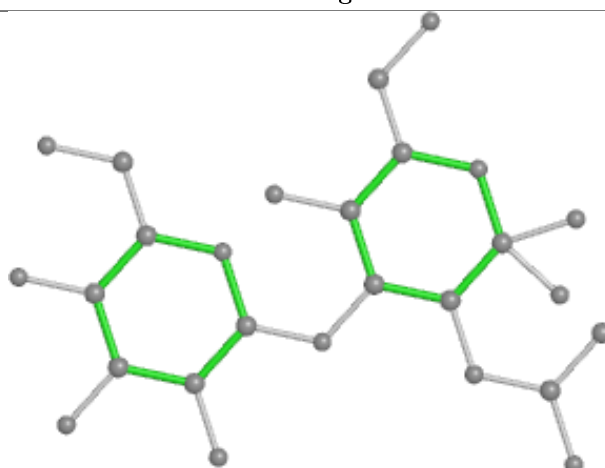
Bond lengths



Bond angles

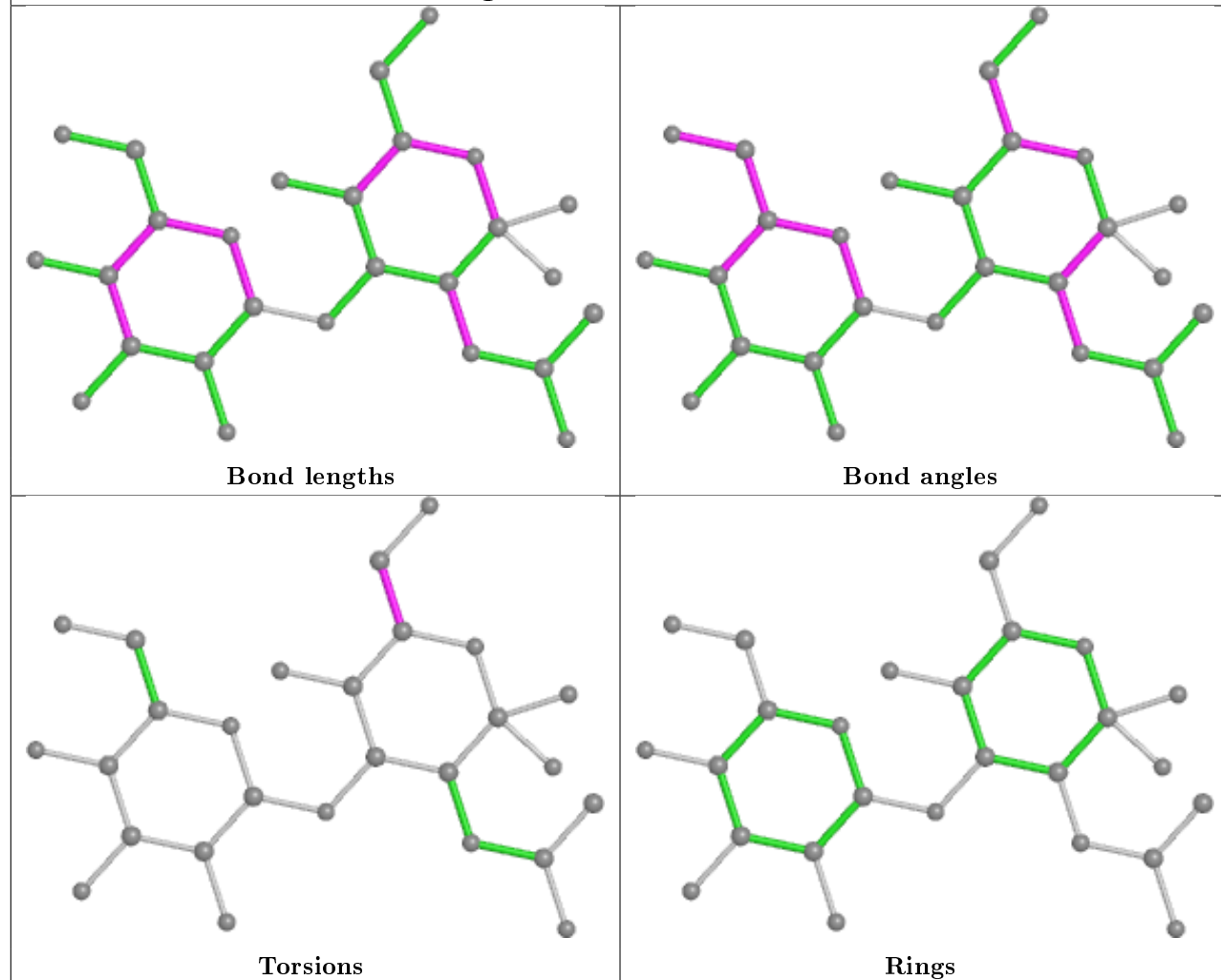


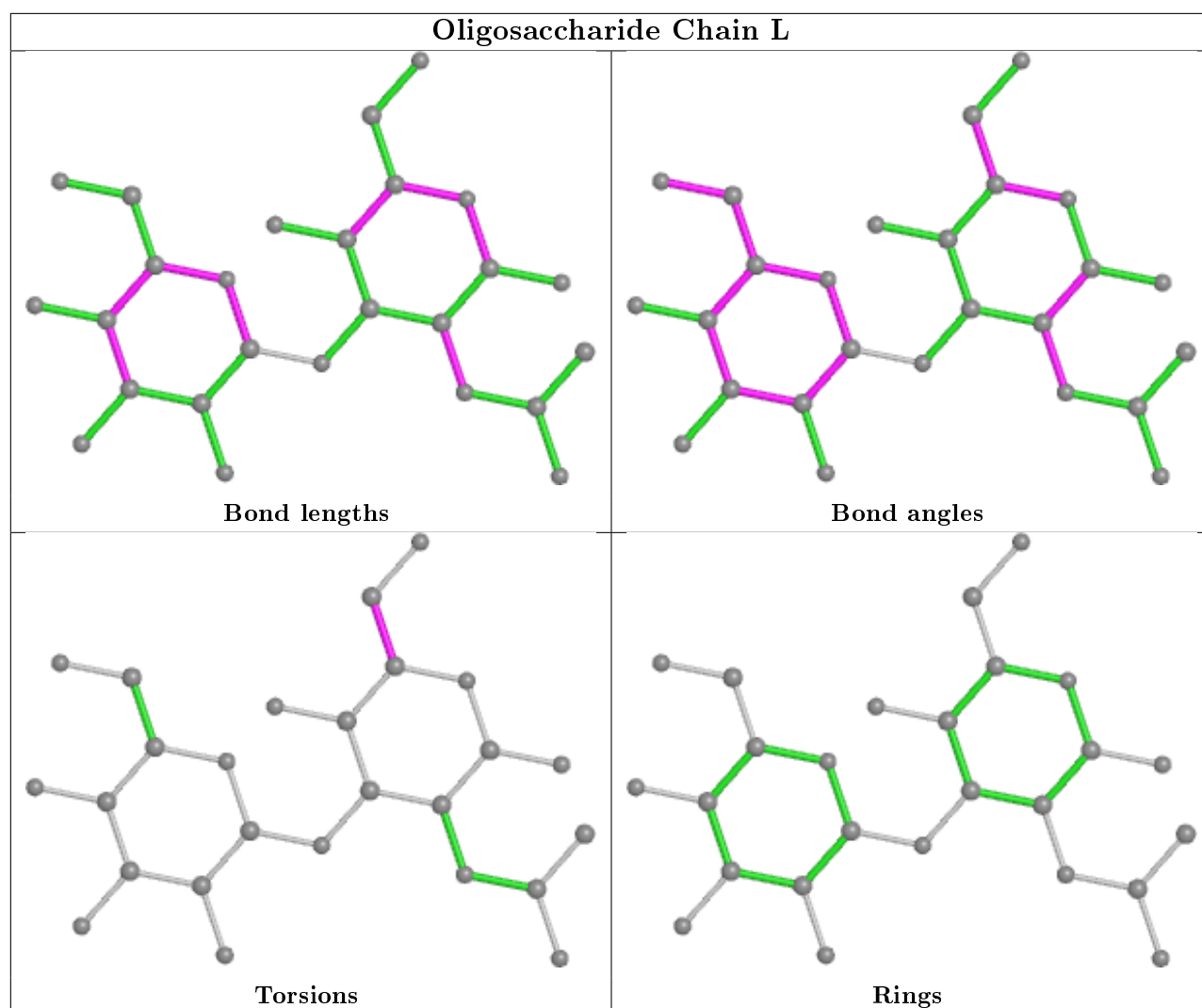
Torsions



Rings

## Oligosaccharide Chain K





## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	133/133 (100%)	-0.14	1 (0%) 86 86	14, 20, 30, 33	0
1	C	133/133 (100%)	-0.11	2 (1%) 73 72	14, 21, 32, 36	0
1	E	133/133 (100%)	-0.19	1 (0%) 86 86	14, 20, 27, 35	0
1	G	133/133 (100%)	-0.09	1 (0%) 86 86	16, 22, 30, 37	0
2	B	15/17 (88%)	0.15	1 (6%) 17 16	16, 20, 32, 43	0
2	D	17/17 (100%)	0.05	2 (11%) 4 3	16, 20, 37, 42	0
2	F	15/17 (88%)	0.06	1 (6%) 17 16	15, 21, 31, 40	0
2	H	15/17 (88%)	0.30	1 (6%) 17 16	18, 22, 38, 47	0
All	All	594/600 (99%)	-0.11	10 (1%) 70 68	14, 21, 32, 47	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	18	LYS	5.2
2	D	20	ALA	3.8
2	F	18	LYS	3.5
2	B	18	LYS	3.5
2	D	18	LYS	2.4
1	C	21	LYS	2.4
1	C	74	ASN	2.2
1	G	21	LYS	2.2
1	A	81	VAL	2.1
1	E	25	ILE	2.1

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

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

### 6.3 Carbohydrates ⓘ

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

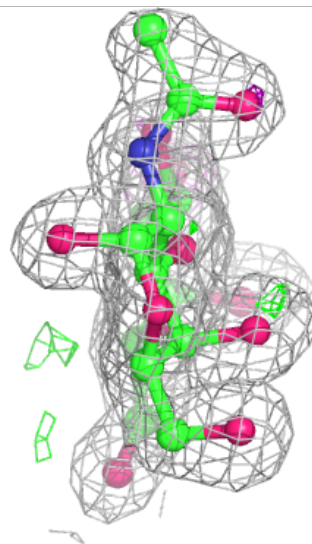
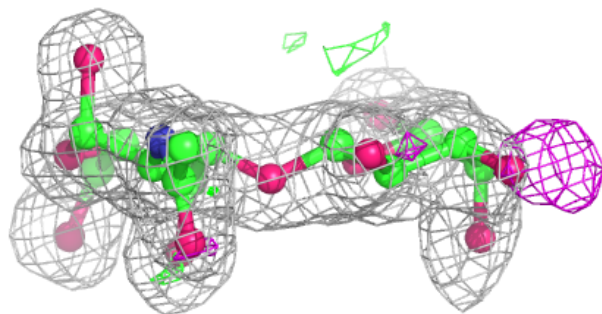
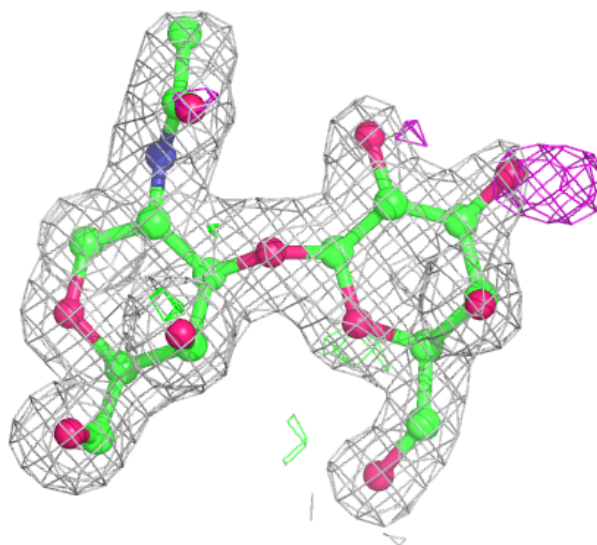
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GAL	I	2	11/12	0.76	0.17	30,33,33,35	0
3	GAL	L	2	11/12	0.80	0.13	33,36,38,38	0
3	GAL	K	2	11/12	0.86	0.12	26,29,31,32	0
3	A2G	L	1	15/15	0.89	0.11	24,28,32,33	0
3	A2G	I	1	15/15	0.92	0.10	17,21,26,27	0
3	A2G	K	1[B]	15/15	0.93	0.10	18,22,29,29	1
3	GAL	J	2	11/12	0.93	0.08	23,24,26,27	0
3	A2G	K	1[A]	15/15	0.93	0.10	18,23,29,29	1
3	A2G	J	1[A]	15/15	0.95	0.08	19,20,26,27	1
3	A2G	J	1[B]	15/15	0.95	0.08	19,21,26,27	1

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.



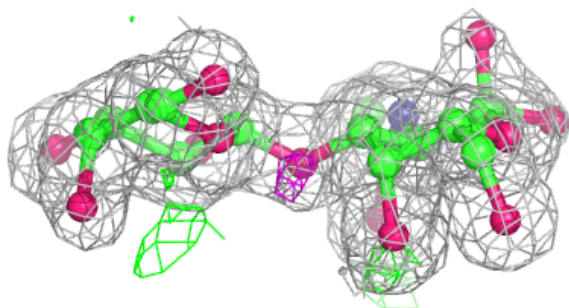
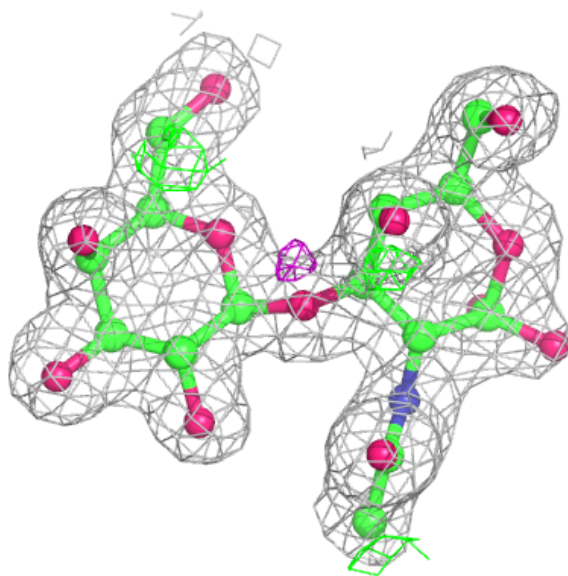
**Electron density around Chain I:**

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



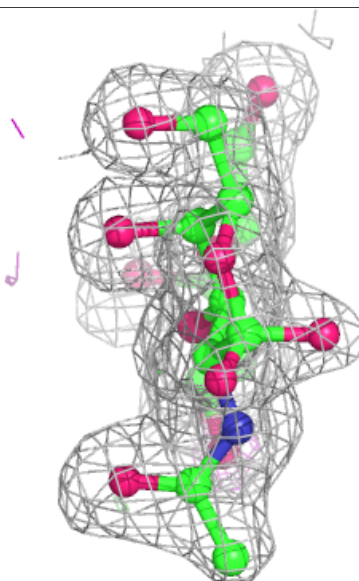
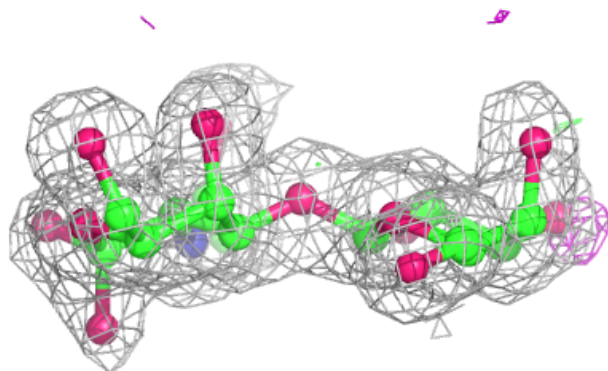
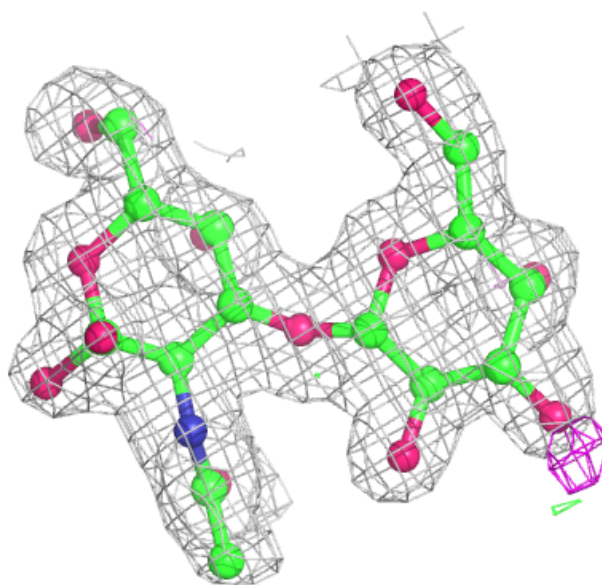
**Electron density around Chain J:**

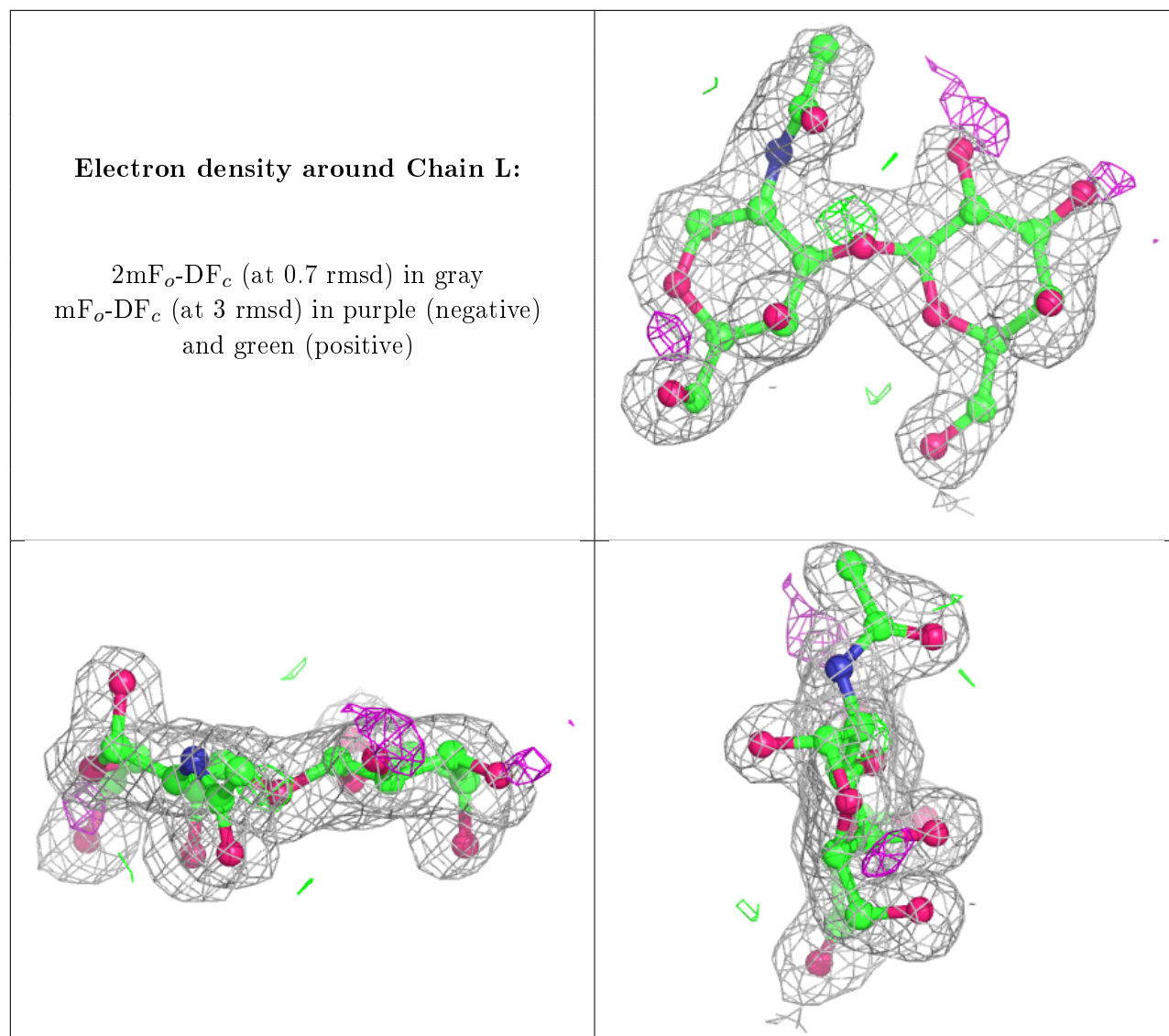
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain K:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.