



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:20 AM GMT

PDB ID : 3AFL  
Title : Crystal structure of exotype alginate lyase Atu3025 H531A complexed with alginate trisaccharide  
Authors : Ochiai, A.; Yamasaki, M.; Mikami, B.; Hashimoto, W.; Murata, K.  
Deposited on : 2010-03-09  
Resolution : 2.99 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

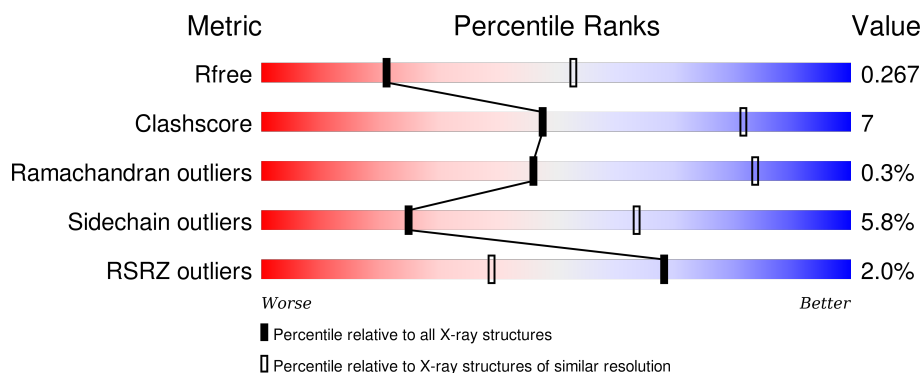
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.99 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	776	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6264 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 Oligo alginate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	766	Total	C	N	O	S	0	2	0
			6166	3936	1063	1153	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	ALA	HIS	ENGINEERED MUTATION	UNP A9CEJ9

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			36	18	18		

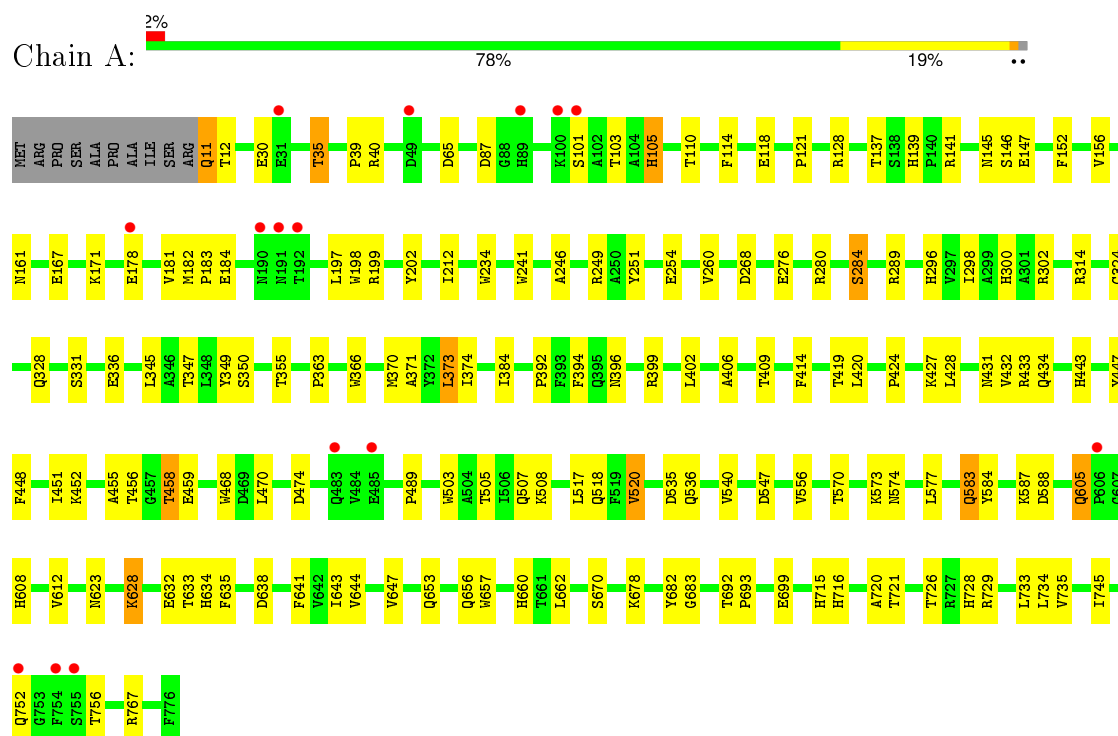
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Oligo alginate lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.84Å 99.64Å 109.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.85 – 2.99 37.85 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.85-2.99) 99.1 (37.85-2.99)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.02 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.199 , 0.262 0.201 , 0.267	Depositor DCC
$R_{free}$ test set	943 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 18422 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MAW, LGU

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	0.42	0/6359	0.54	0/8675

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6166	0	5822	89	0
2	A	36	0	19	2	0
3	A	62	0	0	2	0
All	All	6264	0	5841	89	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 7.

All (89) 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:A:121:PRO:HG2	1:A:392:PRO:HG3	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:GLN:HG2	1:A:583:GLN:HE22	1.41	0.84
1:A:507:GLN:HE22	1:A:518:GLN:HE21	1.25	0.84
1:A:605:GLN:HE21	1:A:608:HIS:HD2	1.35	0.75
1:A:507:GLN:NE2	1:A:518:GLN:HE21	1.88	0.72
1:A:605:GLN:NE2	1:A:608:HIS:HD2	1.88	0.71
1:A:455:ALA:O	1:A:458:THR:HB	1.92	0.69
1:A:406:ALA:H	1:A:518:GLN:HE22	1.41	0.69
1:A:298:ILE:O	1:A:302:ARG:HG2	1.95	0.65
1:A:635:PHE:CZ	1:A:638:ASP:HA	2.32	0.65
1:A:246:ALA:O	1:A:251:TYR:HB3	1.99	0.62
1:A:424:PRO:HB2	1:A:451:ILE:HD12	1.81	0.62
1:A:198:TRP:CH2	2:A:1002:LGU:O3	2.54	0.60
1:A:683:GLY:HA2	1:A:733:LEU:O	2.02	0.59
1:A:608:HIS:HE1	1:A:634:HIS:CD2	2.21	0.59
1:A:535:ASP:HB3	1:A:573:LYS:HG3	1.83	0.58
1:A:612:VAL:HG22	1:A:632:GLU:HG2	1.85	0.58
1:A:520:VAL:HG13	1:A:540:VAL:CG2	2.34	0.58
1:A:656:GLN:HG2	1:A:721:THR:HG23	1.84	0.58
1:A:448:PHE:CZ	1:A:452:LYS:HD2	2.39	0.57
1:A:536:GLN:HG2	1:A:583:GLN:NE2	2.17	0.56
1:A:577:LEU:HB2	1:A:656:GLN:HB2	1.88	0.56
1:A:198:TRP:HH2	2:A:1002:LGU:O3	1.87	0.55
1:A:87:ASP:OD2	1:A:118:GLU:HG2	2.07	0.55
1:A:470:LEU:O	1:A:474:ASP:HB2	2.06	0.55
1:A:657:TRP:HB3	1:A:720:ALA:HB3	1.90	0.54
1:A:409:THR:O	1:A:424:PRO:HD3	2.07	0.54
1:A:280:ARG:O	1:A:284:SER:HB2	2.08	0.54
1:A:40:ARG:HG3	1:A:347:THR:HA	1.89	0.53
1:A:373:LEU:HD21	1:A:394:PHE:CE1	2.43	0.53
1:A:363:PRO:O	1:A:366:TRP:HB3	2.08	0.53
1:A:254:GLU:CD	1:A:314:ARG:HH22	2.12	0.53
1:A:396:ASN:HD22	1:A:399:ARG:HH21	1.57	0.53
1:A:199:ARG:HA	1:A:202:TYR:CE2	2.44	0.52
1:A:254:GLU:OE1	1:A:314:ARG:NH2	2.43	0.52
1:A:733:LEU:HD21	1:A:745:ILE:HB	1.92	0.51
1:A:184:GLU:HB2	1:A:241:TRP:CD1	2.45	0.51
1:A:101:SER:OG	1:A:103:THR:HG22	2.10	0.51
1:A:452:LYS:O	1:A:456:THR:HG23	2.11	0.51
1:A:641:PHE:HB2	1:A:734:LEU:HB2	1.92	0.50
1:A:443:HIS:HD2	1:A:489:PRO:HA	1.75	0.50
1:A:35:THR:HG21	1:A:355:THR:OG1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:HIS:CD2	1:A:489:PRO:HA	2.46	0.50
1:A:145:ASN:OD1	1:A:147:GLU:HG2	2.13	0.49
1:A:402:LEU:HD12	1:A:447:TYR:CD1	2.48	0.49
1:A:574:ASN:HD21	1:A:660:HIS:H	1.61	0.48
1:A:508:LYS:HB2	1:A:517:LEU:HB3	1.95	0.48
1:A:105:HIS:O	1:A:105:HIS:CG	2.66	0.48
1:A:507:GLN:NE2	1:A:518:GLN:HG3	2.27	0.48
1:A:366:TRP:CE2	1:A:370:MET:HG3	2.49	0.47
1:A:574:ASN:ND2	1:A:660:HIS:H	2.12	0.47
1:A:414:PHE:HB2	1:A:503:TRP:CH2	2.50	0.47
1:A:39:PRO:HG2	1:A:114:PHE:CE1	2.50	0.47
1:A:634:HIS:O	1:A:641:PHE:HA	2.15	0.46
1:A:692:THR:HA	1:A:693:PRO:HD3	1.82	0.46
1:A:324:CYS:O	1:A:328:GLN:HG2	2.14	0.46
1:A:623:ASN:HD21	1:A:653:GLN:HE21	1.63	0.45
1:A:632:GLU:HB2	1:A:644:VAL:HB	1.99	0.45
1:A:608:HIS:CE1	1:A:634:HIS:HD2	2.36	0.44
1:A:373:LEU:CD2	1:A:394:PHE:CE1	3.01	0.44
1:A:605:GLN:NE2	1:A:608:HIS:CD2	2.77	0.44
1:A:260:VAL:HG22	1:A:289:ARG:HB3	1.98	0.44
1:A:662:LEU:HD23	1:A:715:HIS:CD2	2.52	0.44
1:A:139:HIS:HD2	1:A:268:ASP:OD1	2.00	0.43
1:A:505:THR:HG22	1:A:520:VAL:HB	1.99	0.43
1:A:296:HIS:O	1:A:300:HIS:HB2	2.18	0.43
1:A:508:LYS:HD2	1:A:508:LYS:HA	1.84	0.43
1:A:349:TYR:HA	1:A:350:SER:HA	1.73	0.43
1:A:574:ASN:ND2	1:A:660:HIS:HD2	2.16	0.43
1:A:182:MET:HA	1:A:183:PRO:HD2	1.94	0.43
1:A:570:THR:OG1	1:A:583:GLN:HG3	2.19	0.42
1:A:181:VAL:HA	1:A:234:TRP:CZ2	2.55	0.42
1:A:128:ARG:NH1	1:A:336:GLU:OE2	2.52	0.42
1:A:633:THR:HG22	1:A:643:ILE:HG12	2.02	0.42
1:A:431:ASN:O	1:A:434:GLN:HB3	2.19	0.42
1:A:345:LEU:HA	1:A:349:TYR:HB2	2.02	0.42
1:A:682:TYR:CE2	1:A:735:VAL:HB	2.54	0.42
1:A:647:VAL:HB	1:A:728:HIS:HB2	2.00	0.42
1:A:11:GLN:N	3:A:2033:HOH:O	2.52	0.41
1:A:628:LYS:HG3	3:A:2030:HOH:O	2.20	0.41
1:A:374:ILE:HG12	1:A:434:GLN:HG2	2.03	0.41
1:A:371:ALA:HB1	1:A:427:LYS:HE3	2.03	0.41
1:A:419:THR:O	1:A:420:LEU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LEU:O	1:A:432:VAL:HG23	2.21	0.41
1:A:584:TYR:OH	1:A:588:ASP:HB3	2.21	0.41
1:A:520:VAL:HG13	1:A:540:VAL:HG22	2.01	0.41
1:A:152:PHE:O	1:A:156:VAL:HG23	2.21	0.41
1:A:699:GLU:HG2	1:A:716:HIS:CD2	2.56	0.40
1:A:141:ARG:NH1	1:A:328:GLN:HB2	2.36	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	766/776 (99%)	721 (94%)	43 (6%)	2 (0%)	46 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	SER
1	A	556	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	640/646 (99%)	601 (94%)	39 (6%)	23 61

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	12	THR
1	A	30	GLU
1	A	35	THR
1	A	65	ASP
1	A	105	HIS
1	A	110	THR
1	A	137	THR
1	A	146	SER
1	A	161	ASN
1	A	167	GLU
1	A	171	LYS
1	A	178	GLU
1	A	197	LEU
1	A	212	ILE
1	A	249	ARG
1	A	276	GLU
1	A	284	SER
1	A	373	LEU
1	A	384	ILE
1	A	433	ARG
1	A	458	THR
1	A	459[A]	GLU
1	A	459[B]	GLU
1	A	468	TRP
1	A	520	VAL
1	A	547[A]	ASP
1	A	547[B]	ASP
1	A	583	GLN
1	A	587	LYS
1	A	605	GLN
1	A	628	LYS
1	A	670	SER
1	A	678	LYS
1	A	726	THR
1	A	729	ARG
1	A	752	GLN
1	A	756	THR
1	A	767	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	HIS
1	A	396	ASN
1	A	450	HIS
1	A	507	GLN
1	A	518	GLN
1	A	559	ASN
1	A	574	ASN
1	A	583	GLN
1	A	605	GLN
1	A	608	HIS
1	A	634	HIS
1	A	653	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 ⓘ

3 carbohydrates 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	LGU	A	1001	2	10,13,13	1.40	1 (10%)	15,19,19	0.93	2 (13%)
2	LGU	A	1002	2	9,12,13	1.24	2 (22%)	13,17,19	1.26	1 (7%)
2	MAW	A	1003	2	7,11,12	2.43	2 (28%)	8,15,17	2.21	2 (25%)

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	LGU	A	1001	2	-	0/0/24/24	0/1/1/1
2	LGU	A	1002	2	-	0/0/21/24	0/1/1/1
2	MAW	A	1003	2	-	0/0/17/20	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	LGU	O5-C1	2.03	1.47	1.43
2	A	1002	LGU	O5-C5	2.55	1.46	1.43
2	A	1001	LGU	O5-C1	2.97	1.48	1.43
2	A	1003	MAW	C3-C4	3.08	1.54	1.50
2	A	1003	MAW	C4-C5	5.32	1.40	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003	MAW	O5-C1-C2	-5.75	104.35	111.06
2	A	1003	MAW	C1-O5-C5	-2.15	110.54	115.30
2	A	1001	LGU	O4-C4-C5	2.08	114.34	110.42
2	A	1001	LGU	O5-C5-C4	2.18	112.48	108.76
2	A	1002	LGU	C6-C5-C4	2.51	120.08	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	LGU	2	0

## 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 ⓘ

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	766/776 (98%)	-0.03	15 (1%) 68 39	25, 37, 50, 66	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	754	PHE	5.5
1	A	192	THR	3.2
1	A	191	ASN	3.0
1	A	100	LYS	3.0
1	A	752	GLN	2.8
1	A	190	ASN	2.7
1	A	178	GLU	2.6
1	A	483	GLN	2.6
1	A	755	SER	2.5
1	A	101	SER	2.4
1	A	485	GLU	2.4
1	A	49	ASP	2.4
1	A	89	HIS	2.4
1	A	606	PRO	2.2
1	A	31	GLU	2.0

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

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

### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LGU	A	1002	12/13	0.88	0.24	0.85	44,46,49,50	0
2	LGU	A	1001	13/13	0.87	0.24	0.54	51,55,56,56	0
2	MAW	A	1003	11/12	0.93	0.20	0.45	41,41,42,43	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.