



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:35 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

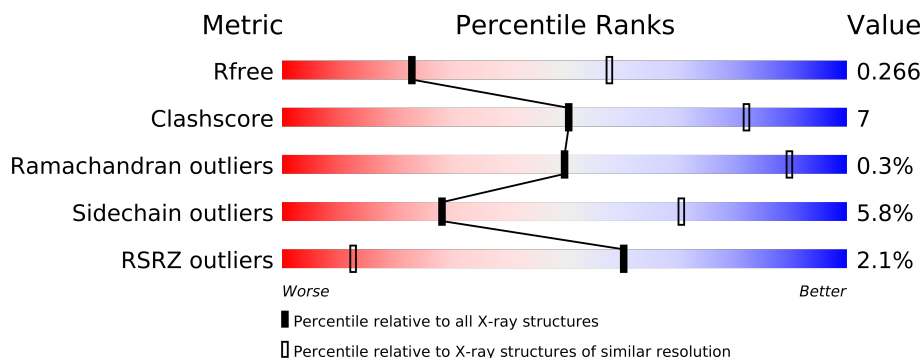
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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		

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 3 is water.

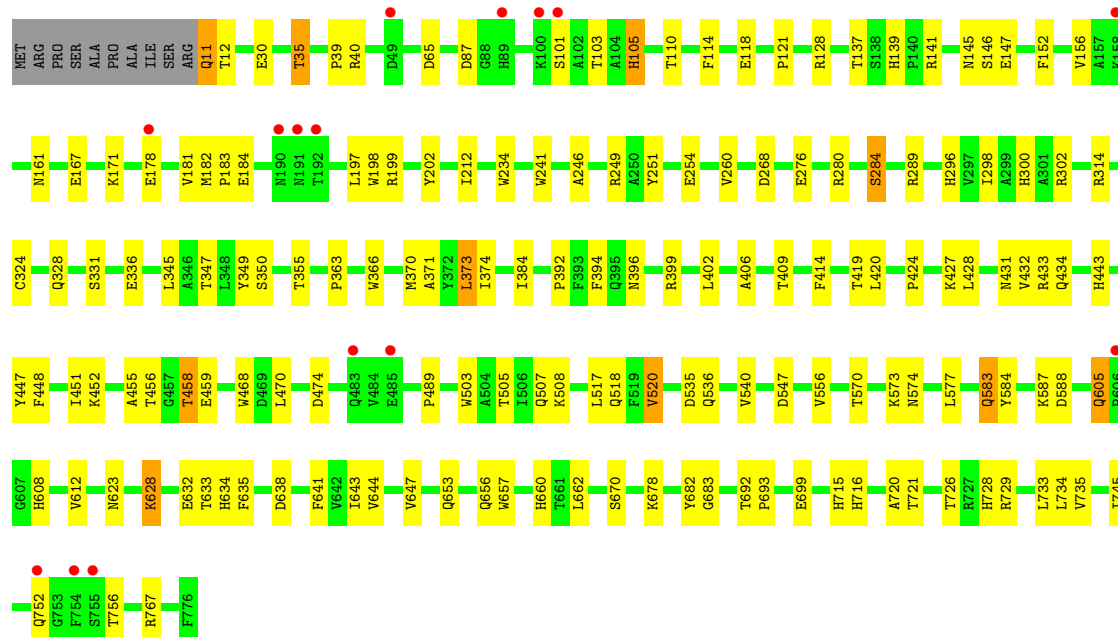
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		

3 Residue-property plots

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

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	5.02 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.262 0.202 , 0.266	Depositor DCC
R_{free} test set	943 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 4.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (89) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:121:PRO:HG2	1:A:392:PRO:HG3	1.55	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:443:HIS:CD2	1:A:489:PRO:HA	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	766/776 (99%)	721 (94%)	43 (6%)	2 (0%)	50	90

All (2) Ramachandran outliers are listed below:

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

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	640/646 (99%)	601 (94%)	39 (6%)	26	68

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

Mol	Chain	Res	Type
1	A	11	GLN
1	A	12	THR

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Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
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 chains 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	13,13,13	1.28	1 (7%)	19,19,19	1.09	1 (5%)
2	LGU	A	1002	2	11,12,13	0.80	0	13,17,19	1.92	2 (15%)
2	MAW	A	1003	2	10,11,12	1.71	2 (20%)	11,15,17	1.61	1 (9%)

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	-	0/4/24/24	1/1/1/1
2	LGU	A	1002	2	-	0/4/21/24	1/1/1/1
2	MAW	A	1003	2	-	0/4/17/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	MAW	C4-C5	3.48	1.40	1.33
2	A	1003	MAW	C3-C4	3.01	1.54	1.50
2	A	1001	LGU	O5-C1	2.80	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	LGU	C4-C5-C6	5.26	120.08	110.84
2	A	1003	MAW	O5-C5-C6	3.94	117.97	111.75
2	A	1002	LGU	C4-C3-C2	2.11	113.33	110.50
2	A	1001	LGU	C4-C5-C6	2.04	114.42	110.84

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	LGU	C1-C2-C3-C4-C5-O5
2	A	1002	LGU	C1-C2-C3-C4-C5-O5

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 95th 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 ²)	Q<0.9
1	A	766/776 (98%)	-0.01	15 (1%) 62 12	25, 37, 50, 66	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	754	PHE	6.1
1	A	192	THR	3.4
1	A	100	LYS	3.2
1	A	755	SER	2.7
1	A	752	GLN	2.7
1	A	483	GLN	2.6
1	A	178	GLU	2.5
1	A	191	ASN	2.5
1	A	190	ASN	2.5
1	A	89	HIS	2.4
1	A	606	PRO	2.4
1	A	49	ASP	2.4
1	A	485	GLU	2.3
1	A	101	SER	2.0
1	A	158	LYS	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, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	LGU	A	1002	12/13	0.24	0.79	44,46,49,50	0
2	MAW	A	1003	11/12	0.20	0.38	41,41,42,43	0
2	LGU	A	1001	13/13	0.22	0.14	51,55,56,56	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.