

Full wwPDB X-ray Structure Validation Report (i)

Jul 6, 2022 - 04:08 pm BST

PDB ID	:	7QOE
Title	:	Structure of a small alarmone hydrolase from Leptospira levettii
Authors	:	Bisiak, F.; Brodersen, D.E.; Chrenkova, A.
Deposited on		
Resolution	:	1.20 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

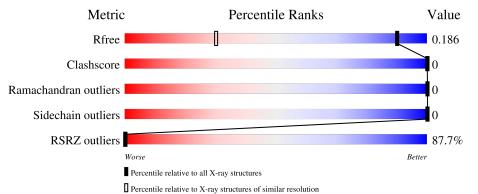
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.20 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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					
			80%					
1	А	204	92%	8%				



7QOE

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3486 atoms, of which 1651 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 HDc domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	187	Total 3262	C 1022	H 1651	N 277	O 308	$\frac{S}{4}$	0	23	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	197	LEU	-	expression tag	UNP A0A2N0AXP5
А	198	GLU	-	expression tag	UNP A0A2N0AXP5
A	199	HIS	-	expression tag	UNP A0A2N0AXP5
А	200	HIS	-	expression tag	UNP A0A2N0AXP5
А	201	HIS	-	expression tag	UNP A0A2N0AXP5
A	202	HIS	-	expression tag	UNP A0A2N0AXP5
А	203	HIS	-	expression tag	UNP A0A2N0AXP5
А	204	HIS	-	expression tag	UNP A0A2N0AXP5

• Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mo	l Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Mn 1 1	0	0

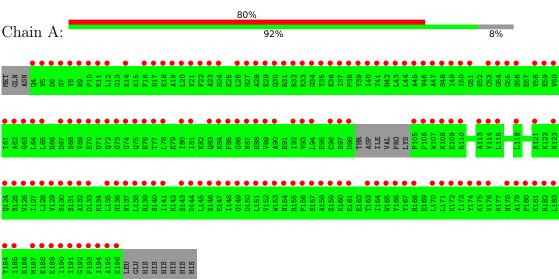
• Molecule 3 is water.

M	ol	Chain	Residues	Atoms		ZeroOcc	AltConf
3		А	223	Total 223	O 223	0	0



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: HDc domain-containing protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants	98.71Å 98.71Å 40.09Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.14 - 1.20	Depositor
	44.14 - 1.20	EDS
% Data completeness	99.6 (44.14 - 1.20)	Depositor
(in resolution range)	$100.0 \ (44.14-1.20)$	EDS
R _{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.41 (at 1.20 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.152 , 0.181	Depositor
It, Itfree	0.160 , 0.186	DCC
R_{free} test set	3120 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	19.9	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ L > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3486	wwPDB-VP
Average B, all atoms $(Å^2)$	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.53% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: MN

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).

Mal	Chain	Bond	lengths	Bond angles		
IVI01	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.34	0/1704	0.57	0/2288	

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	А	1611	1651	1572	0	0
2	А	1	0	0	0	0
3	А	223	0	0	0	0
All	All	1835	1651	1572	0	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 0.

There are no clashes within the asymmetric unit.

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	А	205/204~(100%)	203~(99%)	2(1%)	0	100 100

There are no Ramachandran outliers to report.

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 0		Outliers	Percentiles	
1	А	184/181~(102%)	184 (100%)	0	100 100	

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	А	187/204~(91%)	3.66	164 (87%) 0 0	17, 24, 39, 54	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	194	ILE	12.3
1	А	5	VAL	12.0
1	А	8	TYR	11.0
1	А	98	ASP	10.9
1	А	94	LEU	9.3
1	А	105	PRO	7.4
1	А	193	PHE	6.6
1	А	176	VAL	6.6
1	А	148	ILE	6.3
1	А	152	VAL	6.1
1	А	167	TYR	5.9
1	А	50	ILE	5.9
1	А	40	ILE	5.8
1	А	20	LEU	5.8
1	А	37[A]	ILE	5.6
1	А	156	PHE	5.6
1	А	69	VAL	5.6
1	А	43	LEU	5.6
1	А	155	ARG	5.6
1	А	61	ILE	5.5
1	А	58	VAL	5.5
1	А	138	LEU	5.4
1	А	80	ILE	5.4
1	А	96	CYS	5.4
1	А	109	GLU	5.3
1	А	60	VAL	5.3
1	А	53	CYS	5.2



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\mathbf{Mol}	Chain	Res	Type	RSRZ			
1	А	31[A]	ARG	5.2			
1	А	129	VAL	5.2			
1	А	85	PHE	5.2			
1	А	9	ARG	5.1			
1	А	49	ILE	5.1			
1	А	65	LEU	5.1			
1	А	189[A]	GLU	5.1			
1	А	145	LEU	5.0			
1	А	7	SER	4.9			
1	А	45	ALA	4.8			
1	А	74	GLY	4.8			
1	А	174	TYR	4.7			
1	А	64	LEU	4.7			
1	А	46	VAL	4.6			
1	А	147	GLU	4.6			
1	А	4	GLN	4.6			
1	А	19[A]	ALA	4.6			
1	А	114	TYR	4.5			
1	А	6	ASP	4.5			
1	А	16	PHE	4.5			
1	А	39	TYR	4.5			
1	А	151	LEU	4.4			
1	А	81	ILE	4.4			
1	А	170	LEU	4.3			
1	А	127	ILE	4.3			
1	А	78	LEU	4.3			
1	А	171	LEU	4.3			
1	А	54	GLY	4.3			
1	А	21	VAL	4.3			
1	А	195	ALA	4.3			
1	А	89	VAL	4.2			
1	А	12	LEU	4.2			
1	А	126	VAL	4.2			
1	А	62	ALA	4.2			
1	А	47	ALA	4.1			
1	А	135	LEU	4.1			
1	А	22	PHE	4.1			
1	А	128	LEU	4.0			
1	А	23	ALA	4.0			
1	А	179[A]	ALA	4.0			
1	А	92	ILE	4.0			
1	А	93	VAL	3.9			



Mol Chain		$\frac{1 \text{ previou}}{\text{Res}}$	Type	RSRZ
1	А	164	ILE	3.9
1	А	185	ILE	3.9
1	А	163	THR	3.9
1	А	10	PRO	3.9
1	А	115	LEU	3.9
1	А	178[A]	ASN	3.8
1	А	149	GLY	3.7
1	А	132	ALA	3.7
1	А	38	PRO	3.6
1	А	192	GLY	3.6
1	А	165	TRP	3.6
1	А	106	PRO	3.6
1	А	29	GLU	3.6
1	А	107	TRP	3.5
1	А	184	THR	3.5
1	А	44	LEU	3.5
1	А	110	ARG	3.4
1	А	196	LYS	3.5
1	А	41	THR	3.4
1	А	55	GLY	3.4
1	А	63	GLY	3.4
1	А	118	LEU	3.4
1	А	190[A]	ILE	3.4
1	А	172	LYS	3.3
1	А	24	SER	3.3
1	А	35	THR	3.3
1	А	75	GLN	3.3
1	А	158	ALA	3.3
1	А	11	LYS	3.3
1	А	76	GLU	3.3
1	А	72	GLN	3.2
1	А	140	SER	3.2
1	А	36	GLU	3.2
1	А	70	GLU	3.2
1	А	141	ILE	3.2
1	А	113	ALA	3.2
1	А	183	LEU	3.2
1	А	73	GLY	3.2
1	А	150	ASP	3.1
1	А	87	ASN	3.1
1	А	32[A]	ARG	3.0
1	А	26	LEU	3.0

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Mol Chain		Res	Type	RSRZ
1	А	90	ALA	3.0
1	А	168[A]	ARG	3.0
1	А	166	TYR	3.0
1	А	187[A]	MET	3.0
1	А	28	ALA	3.0
1	А	181[A]	LYS	2.9
1	А	125	SER	2.9
1	А	124	GLN	2.9
1	А	86	GLY	2.9
1	А	173	ILE	2.9
1	А	14[A]	LYS	2.8
1	А	157[A]	SER	2.8
1	А	161[A]	GLU	2.8
1	А	180	PRO	2.8
1	А	77	THR	2.7
1	А	123	ASN	2.7
1	А	51	GLY	2.7
1	А	48	SER	2.7
1	А	56	SER	2.7
1	А	121[A]	SER	2.7
1	А	136	HIS	2.6
1	А	42	HIS	2.6
1	А	27	HIS	2.6
1	А	67	ASP	2.6
1	А	33	LYS	2.5
1	А	68[A]	SER	2.5
1	А	108[A]	LYS	2.4
1	А	146	SER	2.4
1	А	83	GLN	2.4
1	А	191	ILE	2.3
1	А	153	TRP	2.3
1	А	17	ASN	2.3
1	А	34	GLY	2.3
1	А	97	SER	2.3
1	А	71	ASP	2.3
1	А	133	ASP	2.3
1	А	143	SER	2.2
1	A	188[A]	GLU	2.2
1	А	160	LYS	2.2
1	A	139	ARG	2.2
1	A	159	SER	2.2
1	А	175	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	А	30	GLN	2.2
1	А	130	SER	2.1
1	А	137	ASN	2.1
1	А	144	ASP	2.1
1	А	154	ASN	2.1
1	А	182[A]	ARG	2.1
1	А	59	GLU	2.1
1	А	84	LYS	2.1
1	А	88	GLU	2.1
1	А	131	SER	2.1
1	А	18[A]	GLU	2.0

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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)

There are no monosaccharides in this entry.

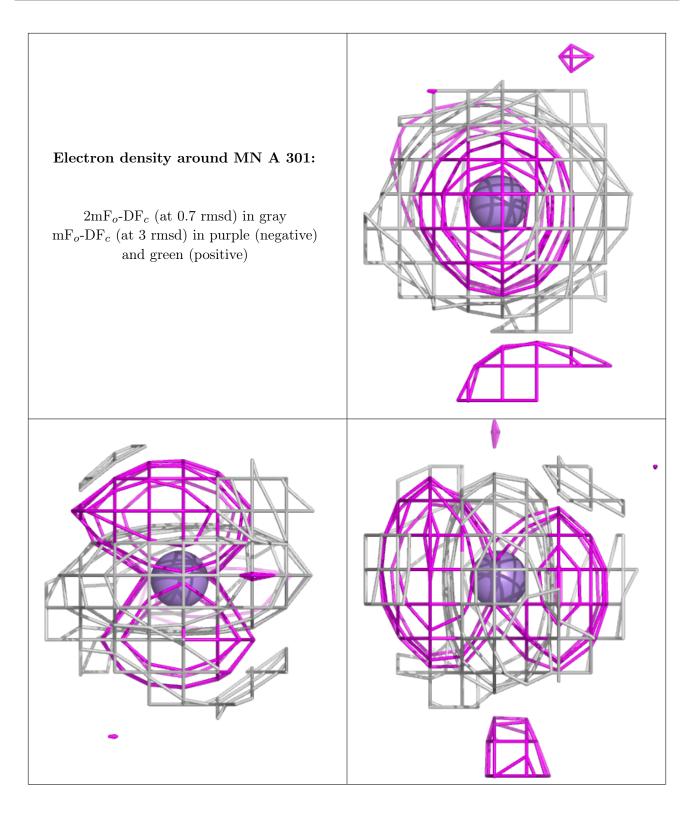
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	$B-factors(A^2)$	Q<0.9
2	MN	А	301	1/1	0.97	0.17	$17,\!17,\!17,\!17$	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

There are no such residues in this entry.

