

# Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 01:39 am BST

PDB ID 6IS3

> Title Crystal Structure of Staphylococcus aureus response regulator ArlR receiver

> > domain

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Deposited on 2018-11-15

1.55 Å(reported) Resolution

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

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

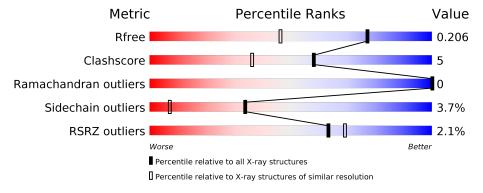
Validation Pipeline (wwPDB-VP) 2.11

## 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 1.55 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
$R_{free}$	130704	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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 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		
1	A	126	87%	7%	• 6%
1	С	126	80%	16%	

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
3	MES	A	202	_	_	_	X



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4146 atoms, of which 1954 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 Response regulator ArlR.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	С	121	Total 1947			± 1	O 193	S 2	0	0	0
1	A	119	Total 1951			N 162	O 193	S 2	0	2	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	-6	MET	-	initiating methionine	UNP Q2YY03
С	-5	GLY	_	expression tag	UNP Q2YY03
С	-4	HIS	_	expression tag	UNP Q2YY03
С	-3	HIS	_	expression tag	UNP Q2YY03
С	-2	HIS	_	expression tag	UNP Q2YY03
С	-1	HIS	_	expression tag	UNP Q2YY03
С	0	HIS	_	expression tag	UNP Q2YY03
С	1	HIS	_	expression tag	UNP Q2YY03
A	-6	MET	_	initiating methionine	UNP Q2YY03
A	-5	GLY	_	expression tag	UNP Q2YY03
A	-4	HIS	_	expression tag	UNP Q2YY03
A	-3	HIS	_	expression tag	UNP Q2YY03
A	-2	HIS		expression tag	UNP Q2YY03
A	-1	HIS	=	expression tag	UNP Q2YY03
A	0	HIS	-	expression tag	UNP Q2YY03
A	1	HIS	-	expression tag	UNP Q2YY03

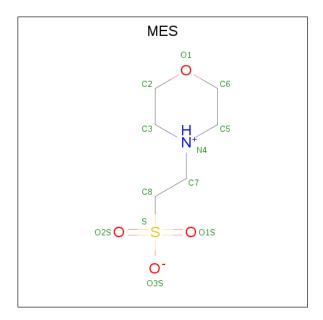
• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	1	Total Ca 1 1	0	0

• Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES)



 $(formula:\ C_6H_{13}N\,O_4S).$ 



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
3	A	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0

#### • Molecule 4 is water.

N	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	4	С	107	Total O 107 107	0	0
	4	A	115	Total O 115 115	0	0



# 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 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: Response regulator ArlR





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	38.38Å 41.21Å 42.88Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.50° 118.85° 96.06°	Depositor
Resolution (Å)	33.00 - 1.55	Depositor
resolution (A)	36.73 - 1.55	EDS
% Data completeness	87.3 (33.00-1.55)	Depositor
(in resolution range)	87.3 (36.73-1.55)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.44 (at 1.55Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
D D.	0.173 , 0.206	Depositor
$R, R_{free}$	0.175 , $0.206$	DCC
$R_{free}$ test set	2000 reflections $(7.04\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38, 47.5	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4146	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.29% of the height of the origin peak. No significant pseudotranslation is detected.

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



<sup>&</sup>lt;sup>1</sup>Intensities 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: CA, MES

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z >5	
1	A	0.41	0/996	0.60	0/1349	
1	С	0.43	0/996	0.63	0/1351	
All	All	0.42	0/1992	0.62	0/2700	

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	976	975	980	5	0
1	С	981	966	968	13	0
2	С	1	0	0	0	0
3	A	12	13	12	4	0
4	A	115	0	0	3	3
4	С	107	0	0	7	1
All	All	2192	1954	1960	19	3

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 5.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance } (\text{\AA}) \end{array}$	Clash overlap (Å)
1:C:11:GLN:NE2	4:C:303:HOH:O	2.16	0.79
1:C:27:ASN:OD1	4:C:301:HOH:O	2.05	0.74
1:C:-1:HIS:O	4:C:302:HOH:O	2.08	0.70
1:A:66:LYS:NZ	4:A:304:HOH:O	2.33	0.60
1:C:4:ILE:HD12	1:C:26:TYR:HB3	1.85	0.57
1:C:65:ARG:NE	4:C:309:HOH:O	2.37	0.57
1:C:29:ASP:OD1	4:C:304:HOH:O	2.19	0.53
1:A:61:LEU:HD22	1:A:93:TYR:CD1	2.46	0.50
1:C:96:ASP:O	3:A:202:MES:H21	2.12	0.49
1:A:39:ASP:OD1	4:A:301:HOH:O	2.20	0.48
1:C:58:ILE:HD11	1:C:62:GLU:HG3	1.94	0.48
1:C:96:ASP:O	3:A:202:MES:H31	2.14	0.48
1:C:104:ASP:HB2	4:C:332:HOH:O	2.13	0.47
1:C:79:THR:HG21	1:C:98:TYR:CE2	2.52	0.44
1:C:119:GLN:O	4:C:305:HOH:O	2.20	0.43
1:A:96:ASP:O	3:A:202:MES:H52	2.19	0.42
3:A:202:MES:H81	4:A:330:HOH:O	2.20	0.41
1:C:6:ILE:HD11	1:C:21:LEU:HD12	2.03	0.41
1:A:56:PRO:O	1:A:57:SER:HB2	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
4:A:407:HOH:O	4:A:413:HOH:O[1_656]	2.01	0.19
4:C:382:HOH:O	4:A:391:HOH:O[1_455]	2.10	0.10
4:A:304:HOH:O	4:A:393:HOH:O[1_655]	2.17	0.03

## 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	Perce	$\mathbf{ntiles}$
1	A	119/126~(94%)	116 (98%)	3 (2%)	0	100	100
1	С	119/126~(94%)	117 (98%)	2 (2%)	0	100	100
All	All	$238/252 \ (94\%)$	233 (98%)	5 (2%)	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	Outliers	Percentile	es
1	A	109/113 (96%)	104 (95%)	5 (5%)	27 4	
1	С	107/113 (95%)	103 (96%)	4 (4%)	34 7	
All	All	216/226 (96%)	207 (96%)	9 (4%)	34 5	

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	0	HIS
1	С	10	GLU
1	С	53	LEU
1	С	71	GLN
1	A	1	HIS
1	A	45	TYR
1	A	61	LEU
1	A	82[A]	SER
1	A	82[B]	SER

Some 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 carbohydrates in this entry.

### 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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).

1	ſol	Type	Chain	Res	Link	Bo	nd leng	ths	В	ond ang	les
1	101	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
	3	MES	A	202	-	12,12,12	2.39	1 (8%)	14,16,16	2.22	5 (35%)

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	${ m Res}$	Link	Chirals	Torsions	Rings
3	MES	A	202	-	-	2/6/14/14	0/1/1/1

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
3	A	202	MES	C8-S	-8.03	1.66	1.77

#### All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathbf{Ideal}(^o)$
3	A	202	MES	C5-N4-C3	5.43	121.05	108.83
3	A	202	MES	C7-N4-C3	3.29	119.64	111.23
3	A	202	MES	C2-C3-N4	3.08	114.77	110.10

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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
3	A	202	MES	O1S-S-C8	2.36	109.75	106.92
3	A	202	MES	O2S-S-C8	2.27	109.65	106.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202	MES	C8-C7-N4-C3
3	A	202	MES	N4-C7-C8-S

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	MES	4	0

## 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q < 0.9
1	A	119/126 (94%)	-0.23	1 (0%) 86 88	15, 26, 51, 63	0
1	С	121/126~(96%)	-0.05	4 (3%) 46 53	16, 29, 61, 85	0
All	All	$240/252 \ (95\%)$	-0.14	5 (2%) 63 69	15, 28, 59, 85	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	-1	HIS	2.8
1	A	45	TYR	2.7
1	С	0	HIS	2.5
1	С	57	SER	2.4
1	С	59	ASN	2.2

## 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 carbohydrates 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	MES	A	202	12/12	0.64	0.44	36,77,143,157	0
2	CA	С	202	1/1	0.94	0.05	60,60,60,60	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

