

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

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PDB ID : 5D86

> Title Staphyloferrin B precursor biosynthetic enzyme SbnA Y152F variant

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1.50 Å(reported) Resolution

This is a wwPDB X-ray Structure Validation Summary 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

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

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

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

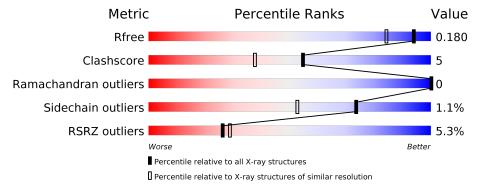
Validation Pipeline (wwPDB-VP) 2.11

## 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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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		
			5%		
1	A	326	86%	11%	••



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3011 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.

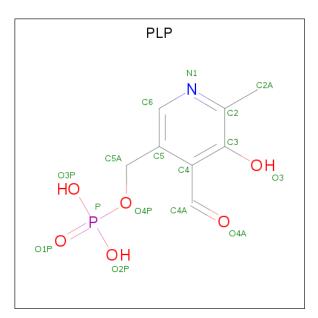
• Molecule 1 is a protein called Probable siderophore biosynthesis protein SbnA.

Mol	Chain	Residues		$\mathbf{At}$	oms			ZeroOcc	AltConf	Trace
1	Λ	318	Total	С	N	О	S	0	23	0
1	A	310	2635	1674	450	496	15	0	23	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	${f Comment}$	Reference
Α	152	PHE	TYR	engineered mutation	UNP A6QDA0

• Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



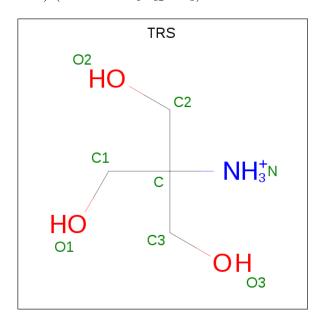
Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf		
2	A	1	Total 15	C 8	N 1	O 5	P 1	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	$\begin{array}{cc} \text{Total} & \text{Mg} \\ 2 & 2 \end{array}$	0	0

• Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
1	Δ	1	Total	С	N	О	0	0
7	11	1	8	4	1	3		

• Molecule 5 is water.

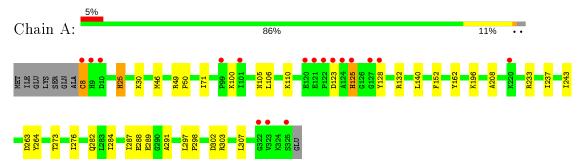
$\mathbf{Mol}$	Chain	Residues	${f Atoms}$	ZeroOcc	$\mathbf{AltConf}$
5	A	351	Total O 351 351	0	0



# 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: Probable siderophore biosynthesis protein SbnA





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	56.36Å 115.99Å 45.45Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.38 - 1.50	Depositor
Resolution (A)	35.38 - 1.50	EDS
% Data completeness	98.1 (35.38-1.50)	Depositor
(in resolution range)	98.1 (35.38-1.50)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$< I/\sigma(I) > 1$	4.40 (at 1.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
D D.	0.148 , 0.180	Depositor
$R, R_{free}$	0.152 , $0.180$	DCC
$R_{free}$ test set	2412 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.7	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36, 50.1	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.29% 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: TRS, MG, PLP

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5	
1	Α	0.64	0/2691	0.74	0/3639	

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	HIS	Sidechain

### 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	2635	0	2674	28	0
2	A	15	0	7	0	0

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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
3	A	2	0	0	0	0
4	A	8	0	12	2	0
5	A	351	0	0	7	1
All	All	3011	0	2693	28	1

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.

The worst 5 of 28 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} & ( ext{Å}) \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:A:233[B]:ARG:NH2	5:A:1103:HOH:O	2.20	0.74
1:A:233[B]:ARG:HG3	1:A:233[B]:ARG:HH11	1.60	0.67
1:A:46:MET:HE2	1:A:298:PRO:HB3	1.77	0.67
1:A:263[B]:ASP:OD2	5:A:1102:HOH:O	2.16	0.59
1:A:100:LYS:O	1:A:100:LYS:HG2	2.03	0.56

All (1) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
5:A:1118:HOH:O	5:A:1380:HOH:O[2_655]	1.99	0.21

### 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	Percentile	es
1	A	338/326 (104%)	326 (96%)	12 (4%)	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	Percentiles	
1	A	$292/276 \ (106\%)$	288 (99%)	4 (1%)	67 42	

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8[A]	CYS
1	A	8[B]	CYS
1	A	125	HIS
1	A	302	ASP

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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).

Mol	Type	Chain	Pag	Res Link		ond leng	ths	Bond angles		
WIOI	Туре	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	TRS	A	1004	-	7,7,7	0.31	0	9,9,9	0.83	0
2	PLP	A	1001	1	15,15,16	1.18	1 (6%)	20,22,23	1.39	3 (15%)

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
4	TRS	A	1004	-	-	3/9/9/9	-
2	PLP	A	1001	1	-	1/6/6/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	${f Observed(\AA)}$	$\operatorname{Ideal}( ext{\AA})$
2	A	1001	PLP	C3-C2	-2.57	1.38	1.40

#### All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^{o})$
2	A	1001	PLP	C5A-C5-C6	-2.70	114.92	119.37
2	A	1001	PLP	C5-C6-N1	-2.35	119.91	123.82
2	A	1001	PLP	C6-C5-C4	2.11	119.81	118.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	PLP	C6-C5-C5A-O4P
4	A	1004	TRS	N-C-C1-O1
4	A	1004	TRS	C2-C-C1-O1
4	A	1004	TRS	C3-C-C1-O1

There are no ring outliers.

1 monomer is involved in 2 short contacts:



Mol	Chain	$\operatorname{Res}$	Type	Clashes	Symm-Clashes
4	A	1004	TRS	2	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.

N.	Iol	Chain	Analysed	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(Å^2)$	Q < 0.9
	1	A	318/326 (97%)	0.03	17 (5%) 26	3 29	7, 13, 34, 67	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	HIS	8.3
1	A	124	ALA	7.1
1	A	8[A]	CYS	3.9
1	A	325	SER	3.4
1	A	220	LYS	3.3

### 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	${f Res}$	Atoms	RSCC	RSR	$oxed{f B-factors({ m \AA}^2)}$	Q<0.9
4	TRS	A	1004	8/8	0.89	0.22	16,40,50,59	0
3	MG	A	1002	1/1	0.96	0.20	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q < 0.9
2	PLP	A	1001	15/16	0.97	0.07	8,10,13,14	0
3	MG	A	1003	1/1	0.97	0.10	22,22,22,22	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

