

wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 04:44 am BST

PDB ID : 4F24

Title: Crystal structures reveal the multi-ligand binding mechanism of the Staphy-

lococcus aureus ClfB

Authors: Yang, M.J.; Xiang, H.; Wang, J.W.; Liu, B.; Chen, Y.G.; Liu, L.; Deng, X.M.;

Feng, Y.

Deposited on : 2012-05-07

Resolution : 2.51 Å(reported)

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 Xtriage (Phenix) : 1.13

EDS : 2.11

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

Refmac: 5.8.0158

 $\begin{array}{cccc} & CCP4 & : & 7.0.044 \; (Gargrove) \\ Ideal \; geometry \; (proteins) & : & Engh \; \& \; Huber \; (2001) \end{array}$

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

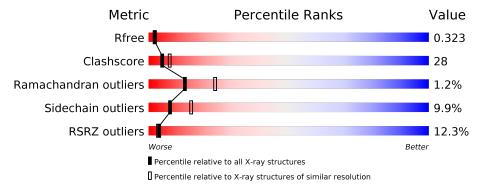
Validation Pipeline (wwPDB-VP) : 2.11

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 2.51 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 $(\# \mathrm{Entries})$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries}, ext{resolution range}(ext{Å})) \end{aligned}$
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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				
			11%				
1	A	363		53%	34%	5%	8%

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
2	MG	A	604	_	_	-	X



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2579 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 Clumping factor B.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	334	Total	С	N	О	S	0	0	0
1	A	354	2574	1613	421	537	3	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	MET	=	EXPRESSION TAG	UNP Q6GDH2
A	181	ARG	=	EXPRESSION TAG	UNP Q6GDH2
A	182	GLY	-	EXPRESSION TAG	UNP Q6GDH2
A	183	SER	-	EXPRESSION TAG	UNP Q6GDH2
A	184	HIS	-	EXPRESSION TAG	UNP Q6GDH2
A	185	HIS	-	EXPRESSION TAG	UNP Q6GDH2
A	186	HIS	=	EXPRESSION TAG	UNP Q6GDH2
A	187	HIS	-	EXPRESSION TAG	UNP Q6GDH2
A	188	HIS	-	EXPRESSION TAG	UNP Q6GDH2
A	189	HIS	-	EXPRESSION TAG	UNP Q6GDH2
A	190	GLU	=	EXPRESSION TAG	UNP Q6GDH2
A	191	ASN	-	EXPRESSION TAG	UNP Q6GDH2
A	192	LEU	-	EXPRESSION TAG	UNP Q6GDH2
A	193	TYR	-	EXPRESSION TAG	UNP Q6GDH2
A	194	PHE		EXPRESSION TAG	UNP Q6GDH2
A	195	GLN	=	EXPRESSION TAG	UNP Q6GDH2
A	196	GLY	-	EXPRESSION TAG	UNP Q6GDH2

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

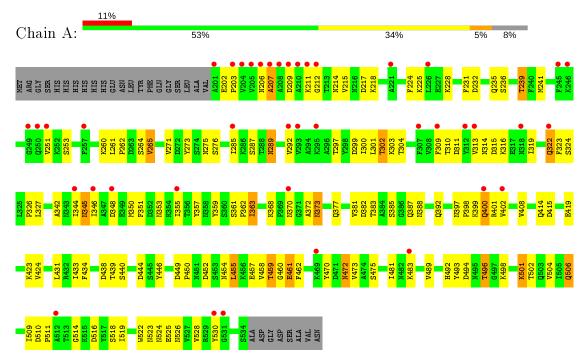
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Mg 5 5	0	0



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: Clumping factor B





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	94.42Å 94.42Å 86.72Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.23 - 2.51	Depositor
Resolution (A)	47.21 - 2.51	EDS
% Data completeness	99.1 (42.23-2.51)	Depositor
(in resolution range)	100.0 (47.21-2.51)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	8.91 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.3_473)	Depositor
P. P.	0.233 , 0.289	Depositor
R, R_{free}	0.270 , 0.323	DCC
R_{free} test set	695 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 57.2	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	0.92	EDS
Total number of atoms	2579	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: MG

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	Mol Chain		lengths	Bond angles		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.44	0/2623	0.56	0/3564	

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	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2574	0	2452	139	2
2	A	5	0	0	0	0
All	All	2579	0	2452	139	2

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 28.

The worst 5 of 139 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	Clash overlap (Å)
1:A:423:LYS:HE3	1:A:494:ASP:CB	1.36	1.53
1:A:423:LYS:CE	1:A:494:ASP:HB3	1.40	1.47

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Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{array}$	Clash overlap (Å)
1:A:423:LYS:HE3	1:A:494:ASP:CA	1.83	1.08
1:A:423:LYS:CE	1:A:494:ASP:CB	2.12	1.04
1:A:433:ILE:H	1:A:459:THR:HG22	1.22	1.04

All (2) 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	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:A:206:ASN:OD1	1:A:519:ILE:O[3_544]	1.72	0.48
1:A:202:GLU:OE1	1:A:377:GLN:NE2[3_544]	1.84	0.36

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	$332/363 \ (92\%)$	309 (93%)	19 (6%)	4 (1%)	13 24	

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	PRO
1	A	207	ALA
1	A	212	GLY
1	A	211	LYS

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	${f Analysed}$	${f Rotameric}$	Outliers	Percentiles		
1	A	283/309 (92%)	255~(90%)	28 (10%)	8 15		

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	THR
1	A	363	ILE
1	A	501	LYS
1	A	322	GLN
1	A	345	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	GLN
1	A	526	ASN
1	A	472	ASN
1	A	377	GLN
1	A	454	ASN

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 5 ligands modelled in this entry, 5 are 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 $>$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	334/363 (92%)	0.85	41 (12%) 4 3	23, 73, 108, 137	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	530	TYR	8.7
1	A	251	VAL	7.2
1	A	211	LYS	5.6
1	A	531	GLY	4.6
1	A	257	PHE	4.3

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	${f B\text{-factors}}({f A}^2)$	$\mathbf{Q}{<}0.9$
2	MG	A	603	1/1	0.58	0.33	84,84,84,84	0
2	MG	A	604	1/1	0.77	0.52	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$ extbf{B-factors}(extbf{A}^2)$	Q < 0.9
2	MG	A	605	1/1	0.83	0.16	85,85,85,85	0
2	MG	A	601	1/1	0.83	0.55	72,72,72,72	0
2	MG	A	602	1/1	0.83	0.81	149,149,149,149	0

6.5 Other polymers (i)

There are no such residues in this entry.

