



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2019 – 02:56 AM EDT

PDB ID : 5OR1
Title : BamA structure of Salmonella enterica
Authors : Dong, C.; Gu, Y.
Deposited on : 2017-08-14
Resolution : 2.92 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.4
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

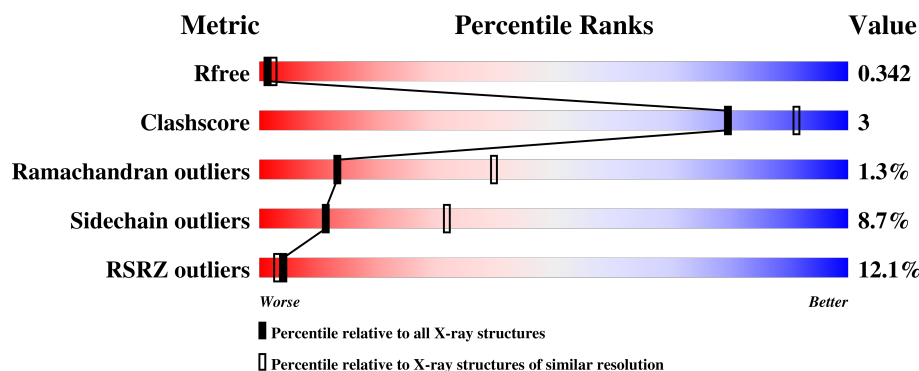
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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}	111664	1983 (2.94-2.90)
Clashscore	122126	2200 (2.94-2.90)
Ramachandran outliers	120053	2150 (2.94-2.90)
Sidechain outliers	120020	2152 (2.94-2.90)
RSRZ outliers	108989	1928 (2.94-2.90)

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. 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 $\leq 5\%$. 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	804	<div> <div>6%</div> <div>41%</div> <div>6%</div> <div>53%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2944 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	380	2944	1860	479	595	10	0	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.04Å 124.04Å 131.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	107.42 – 2.92 62.02 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.7 (107.42-2.92) 99.7 (62.02-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.307 , 0.347 0.308 , 0.342	Depositor DCC
R_{free} test set	666 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	2944	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

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	0.46	0/3028	0.72	2/4121 (0.0%)

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	1	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	489	ILE	N-CA-C	-6.66	93.02	111.00
1	A	724	ASN	CB-CA-C	6.25	122.89	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	720	GLU	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	772	SER	Peptide

5.2 Too-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 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	2944	0	2682	17	0
All	All	2944	0	2682	17	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 3.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:LYS:O	1:A:722:TYR:HB2	1.96	0.65
1:A:479:THR:HG22	1:A:483:VAL:HB	1.84	0.58
1:A:651:GLY:O	1:A:662:ASN:N	2.31	0.54
1:A:630:ARG:HB3	1:A:706:VAL:HG22	1.94	0.49
1:A:723:ALA:N	1:A:724:ASN:HB3	2.29	0.47
1:A:772:SER:HB3	1:A:773:PRO:HD3	1.98	0.46
1:A:543:ILE:HD12	1:A:669:VAL:HB	1.97	0.46
1:A:672:ASN:ND2	1:A:687:CYS:SG	2.90	0.45
1:A:770:TRP:CZ2	1:A:772:SER:HB3	2.52	0.45
1:A:777:LEU:HD21	1:A:779:PHE:CE1	2.52	0.44
1:A:772:SER:CB	1:A:773:PRO:HD3	2.48	0.44
1:A:688:THR:O	1:A:689:GLN:CB	2.66	0.44
1:A:777:LEU:HD21	1:A:779:PHE:CZ	2.54	0.42
1:A:427:ASN:N	1:A:443:GLY:O	2.51	0.41
1:A:745:SER:OG	1:A:746:SER:N	2.54	0.41
1:A:659:PHE:CZ	1:A:761:ARG:HB3	2.56	0.41
1:A:687:CYS:SG	1:A:690:GLU:HB3	2.61	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	378/804 (47%)	337 (89%)	36 (10%)	5 (1%)	13	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	689	GLN
1	A	722	TYR
1	A	724	ASN
1	A	746	SER
1	A	580	GLY

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	310/683 (45%)	283 (91%)	27 (9%)	11	32

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	435	GLU
1	A	446	GLN
1	A	470	GLU
1	A	500	ASP
1	A	514	THR
1	A	523	ASN
1	A	525	LEU
1	A	537	SER
1	A	557	ASP
1	A	558	THR
1	A	595	VAL
1	A	607	VAL
1	A	608	SER
1	A	613	THR
1	A	617	ILE

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Mol	Chain	Res	Type
1	A	629	THR
1	A	657	ARG
1	A	720	GLU
1	A	722	TYR
1	A	730	PHE
1	A	734	MET
1	A	736	THR
1	A	760	ILE
1	A	761	ARG
1	A	771	MET
1	A	772	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	495	GLN
1	A	672	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

There are no carbohydrates in this entry.

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	380/804 (47%)	0.48	46 (12%) ⓘ ⓘ	22, 86, 159, 187	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	785	PHE	11.1
1	A	787	LYS	10.0
1	A	792	LYS	9.3
1	A	793	ALA	8.9
1	A	723	ALA	8.7
1	A	786	LYS	7.5
1	A	794	GLU	7.0
1	A	688	THR	6.8
1	A	789	ASP	6.8
1	A	720	GLU	6.6
1	A	623	TRP	6.6
1	A	619	ASN	6.5
1	A	791	ASP	5.1
1	A	617	ILE	5.0
1	A	682	ASP	4.8
1	A	680	ASP	4.8
1	A	788	TYR	4.3
1	A	783	GLN	4.3
1	A	683	ASP	4.1
1	A	560	SER	4.1
1	A	620	ASP	3.6
1	A	588	ARG	3.5
1	A	724	ASN	3.5
1	A	678	TRP	3.4
1	A	684	TYR	3.4
1	A	790	GLY	3.4
1	A	732	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	730	PHE	3.3
1	A	616	PRO	3.2
1	A	735	GLY	3.0
1	A	784	PRO	3.0
1	A	561	PHE	3.0
1	A	719	SER	2.9
1	A	677	SER	2.8
1	A	722	TYR	2.7
1	A	795	GLN	2.7
1	A	577	LEU	2.5
1	A	621	HIS	2.5
1	A	689	GLN	2.4
1	A	781	TYR	2.3
1	A	685	GLU	2.3
1	A	535	LYS	2.2
1	A	679	ASP	2.2
1	A	599	GLY	2.1
1	A	500	ASP	2.1
1	A	440	PHE	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.