



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 29, 2020 – 12:08 PM JST

PDB ID : 6LYR  
Title : Structure of the BAM complex  
Authors : Xiao, L.; Huang, Y.  
Deposited on : 2020-02-15  
Resolution : 3.28 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](mailto: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.

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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	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

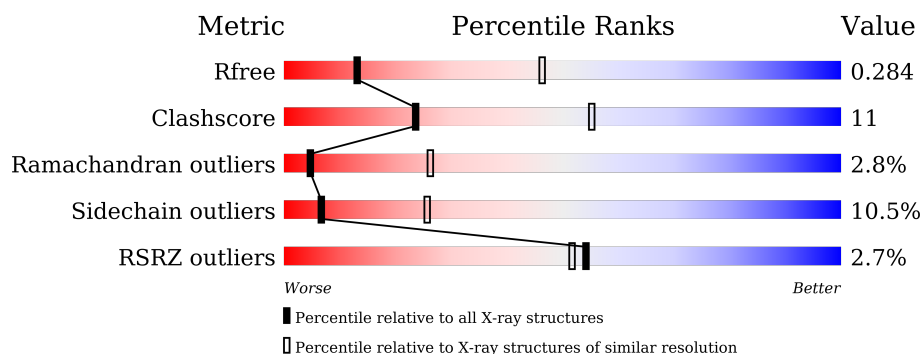
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.28 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))
$R_{free}$	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	810	<div> <div>3%</div> <div>70%</div> <div>23%</div> <div>.</div> <div>.</div> </div>
2	B	400	<div> <div>3%</div> <div>58%</div> <div>28%</div> <div>.</div> <div>11%</div> </div>
3	C	344	<div> <div>12%</div> <div>84%</div> </div>
4	D	245	<div> <div>64%</div> <div>20%</div> <div>15%</div> </div>
5	E	119	<div> <div>2%</div> <div>39%</div> <div>26%</div> <div>8%</div> <div>26%</div> </div>
6	P	9	<div> <div>33%</div> <div>22%</div> <div>33%</div> <div>44%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11439 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
1	A	786	Total	C	N	O	S	0	0	0
			6074	3826	1022	1210	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	760	TRP	TYR	conflict	UNP P0A940

- Molecule 2 is a protein called Outer membrane protein assembly factor BamB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	356	Total	C	N	O	S	0	0	0
			2629	1652	449	522	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	393	TRP	-	expression tag	UNP P77774
B	394	SER	-	expression tag	UNP P77774
B	395	HIS	-	expression tag	UNP P77774
B	396	PRO	-	expression tag	UNP P77774
B	397	GLN	-	expression tag	UNP P77774
B	398	PHE	-	expression tag	UNP P77774
B	399	GLU	-	expression tag	UNP P77774
B	400	LYS	-	expression tag	UNP P77774

- Molecule 3 is a protein called Outer membrane protein assembly factor BamC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	56	Total	C	N	O	S	0	0	0
			378	239	63	75	1			

- Molecule 4 is a protein called Outer membrane protein assembly factor BamD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1642	1035	286	314	7			

- Molecule 5 is a protein called Outer membrane protein assembly factor BamE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	88	Total	C	N	O	S	0	0	0
			657	415	108	132	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	HIS	-	expression tag	UNP P0A937
E	115	HIS	-	expression tag	UNP P0A937
E	116	HIS	-	expression tag	UNP P0A937
E	117	HIS	-	expression tag	UNP P0A937
E	118	HIS	-	expression tag	UNP P0A937
E	119	HIS	-	expression tag	UNP P0A937

- Molecule 6 is a protein called Peptide from Outer membrane protein A.

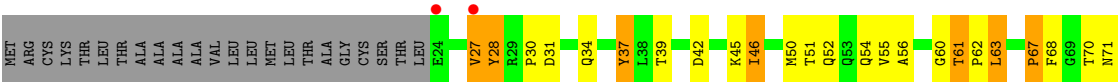
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	P	9	Total	C	N	O	S	0	0	0
			59	36	10	12	1			



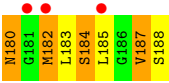
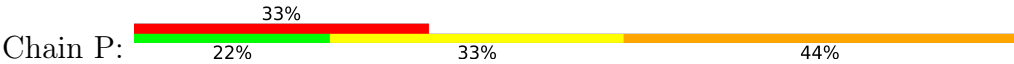
- Molecule 1: Outer membrane protein assembly factor BamA







● Molecule 6: Peptide from Outer membrane protein A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.88Å 116.88Å 430.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 3.28 49.32 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.37-3.28) 99.4 (49.32-3.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.246 , 0.280 0.250 , 0.284	Depositor DCC
$R_{free}$ test set	2302 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.1	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 55.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.64	0/6212	0.78	0/8446
2	B	0.66	0/2674	0.80	0/3652
3	C	0.67	0/387	0.76	0/533
4	D	0.64	0/1678	0.74	0/2285
5	E	0.65	0/671	0.81	0/919
6	P	0.70	0/58	1.57	1/76 (1.3%)
All	All	0.65	0/11680	0.79	1/15911 (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	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	P	184	SER	N-CA-CB	-10.43	94.86	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	722	THR	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	6074	0	5674	123	0
2	B	2629	0	2556	69	0
3	C	378	0	362	11	0
4	D	1642	0	1559	38	0
5	E	657	0	615	24	0
6	P	59	0	61	4	0
All	All	11439	0	10827	250	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 11.

The worst 5 of 250 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:205:TRP:HA	1:A:208:VAL:HG23	1.33	1.07
2:B:223:GLN:HE21	2:B:225:GLN:HB3	1.24	1.02
6:P:183:LEU:HG	6:P:184:SER:N	1.92	0.83
1:A:681:ASN:OD1	1:A:688:TYR:OH	1.95	0.82
1:A:205:TRP:HA	1:A:208:VAL:CG2	2.11	0.80

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	782/810 (96%)	680 (87%)	86 (11%)	16 (2%)	7 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	350/400 (88%)	300 (86%)	35 (10%)	15 (4%)	2	17
3	C	54/344 (16%)	45 (83%)	7 (13%)	2 (4%)	3	20
4	D	204/245 (83%)	189 (93%)	15 (7%)	0	100	100
5	E	86/119 (72%)	66 (77%)	13 (15%)	7 (8%)	1	6
6	P	7/9 (78%)	2 (29%)	4 (57%)	1 (14%)	0	1
All	All	1483/1927 (77%)	1282 (86%)	160 (11%)	41 (3%)	5	26

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	TYR
1	A	697	LYS
2	B	137	SER
2	B	244	LEU
2	B	263	TYR

### 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	638/688 (93%)	563 (88%)	75 (12%)	5	21
2	B	278/329 (84%)	255 (92%)	23 (8%)	11	35
3	C	36/276 (13%)	34 (94%)	2 (6%)	21	51
4	D	166/204 (81%)	159 (96%)	7 (4%)	30	60
5	E	71/101 (70%)	57 (80%)	14 (20%)	1	5
6	P	7/7 (100%)	2 (29%)	5 (71%)	0	0
All	All	1196/1605 (74%)	1070 (90%)	126 (10%)	7	26

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	PHE

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Mol	Chain	Res	Type
1	A	735	THR
5	E	90	THR
1	A	578	TYR
1	A	621	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
2	B	223	GLN
1	A	466	GLN
1	A	259	ASN
1	A	561	GLN

### 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](#)

There are no ligands in this entry.

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	786/810 (97%)	0.09	23 (2%) 51 50	74, 102, 134, 170	0
2	B	356/400 (89%)	0.16	11 (3%) 49 48	75, 103, 132, 160	0
3	C	56/344 (16%)	0.13	1 (1%) 68 66	87, 111, 151, 165	0
4	D	208/245 (84%)	-0.14	1 (0%) 91 91	79, 101, 136, 156	0
5	E	88/119 (73%)	0.02	2 (2%) 60 58	84, 107, 143, 184	0
6	P	9/9 (100%)	1.91	3 (33%) 0 0	133, 153, 160, 163	0
All	All	1503/1927 (77%)	0.09	41 (2%) 54 52	74, 103, 138, 184	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	SER	4.9
1	A	809	THR	4.4
1	A	488	ARG	3.7
6	P	185	LEU	3.6
2	B	295	ARG	3.4

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.