



# wwPDB EM Model Validation Summary Report ⓘ

Jun 4, 2020 – 12:48 PM EDT

PDB ID : 6V05  
EMDB ID : EMD-20969  
Title : Cryo-EM structure of a substrate-engaged Bam complex  
Authors : Tomasek, D.; Rawson, S.; Lee, J.; Wzorek, J.S.; Harrison, S.C.; Li, Z.; Kahne, D.  
Deposited on : 2019-11-18  
Resolution : 4.10 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB 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/EMValidationReportHelp>

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  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.10.1

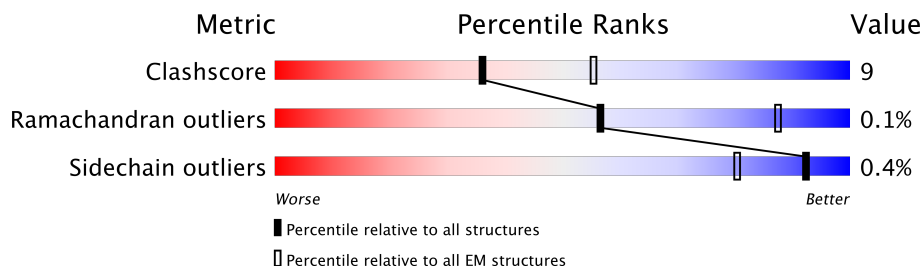
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	810	82% 12% 6%
2	B	392	67% 20% 13%
3	C	344	45% 7% 47%
4	D	245	64% 23% 13%
5	E	123	57% 11% 33%
6	F	578	42% 11% 47%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13705 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	A	758	Total	C	N	O	S	0	0
			5429	3351	961	1104	13		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	690	SER	CYS	engineered mutation	UNP P0A940
A	700	SER	CYS	engineered mutation	UNP P0A940
A	804	CYS	PHE	engineered mutation	UNP P0A940

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	340	Total	C	N	O	S	0	0
			2522	1588	436	492	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	181	Total	C	N	O	S	0	0
			919	516	197	205	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	213	Total	C	N	O	S	0	0
			1722	1086	303	326	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	83	Total	C	N	O	S	0	0
			645	405	112	126	2		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	GLY	-	expression tag	UNP A0A3S5E0E0
E	115	GLY	-	expression tag	UNP A0A3S5E0E0
E	116	HIS	-	expression tag	UNP A0A3S5E0E0
E	117	HIS	-	expression tag	UNP A0A3S5E0E0
E	118	HIS	-	expression tag	UNP A0A3S5E0E0
E	119	HIS	-	expression tag	UNP A0A3S5E0E0
E	120	HIS	-	expression tag	UNP A0A3S5E0E0
E	121	HIS	-	expression tag	UNP A0A3S5E0E0
E	122	HIS	-	expression tag	UNP A0A3S5E0E0
E	123	HIS	-	expression tag	UNP A0A3S5E0E0

- Molecule 6 is a protein called Outer membrane protein assembly factor BamA,Outer membrane protein assembly factor BamA,Outer membrane protein assembly factor BamA,Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	309	Total	C	N	O	S	0	0
			2468	1572	398	489	9		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	254	TRP	-	linker	UNP P0A940
F	255	SER	-	linker	UNP P0A940
F	256	HIS	-	linker	UNP P0A940
F	257	PRO	-	linker	UNP P0A940
F	258	GLN	-	linker	UNP P0A940
F	259	PHE	-	linker	UNP P0A940
F	260	GLU	-	linker	UNP P0A940
F	261	LYS	-	linker	UNP P0A940
F	262	GLY	-	linker	UNP P0A940
F	263	GLY	-	linker	UNP P0A940
F	264	GLY	-	linker	UNP P0A940
F	265	SER	-	linker	UNP P0A940
F	266	GLY	-	linker	UNP P0A940
F	267	GLY	-	linker	UNP P0A940
F	268	GLY	-	linker	UNP P0A940
F	269	SER	-	linker	UNP P0A940
F	270	GLY	-	linker	UNP P0A940
F	271	GLY	-	linker	UNP P0A940
F	272	SER	-	linker	UNP P0A940

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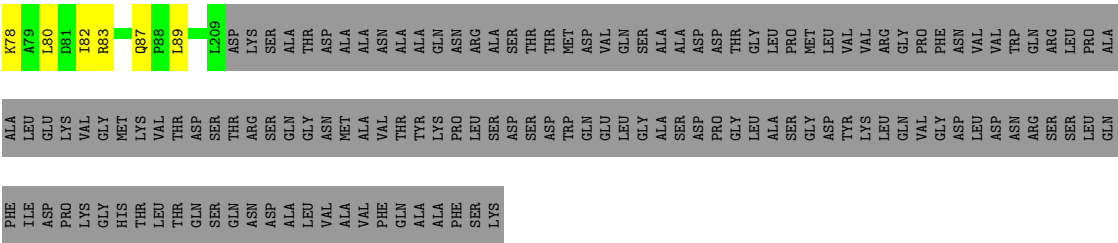
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Chain	Residue	Modelled	Actual	Comment	Reference
F	273	ALA	-	linker	UNP P0A940
F	274	TRP	-	linker	UNP P0A940
F	275	SER	-	linker	UNP P0A940
F	276	HIS	-	linker	UNP P0A940
F	277	PRO	-	linker	UNP P0A940
F	278	GLN	-	linker	UNP P0A940
F	279	PHE	-	linker	UNP P0A940
F	280	GLU	-	linker	UNP P0A940
F	281	LYS	-	linker	UNP P0A940
F	467	CYS	THR	engineered mutation	UNP P0A940
F	690	SER	CYS	engineered mutation	UNP P0A940
F	700	SER	CYS	engineered mutation	UNP P0A940

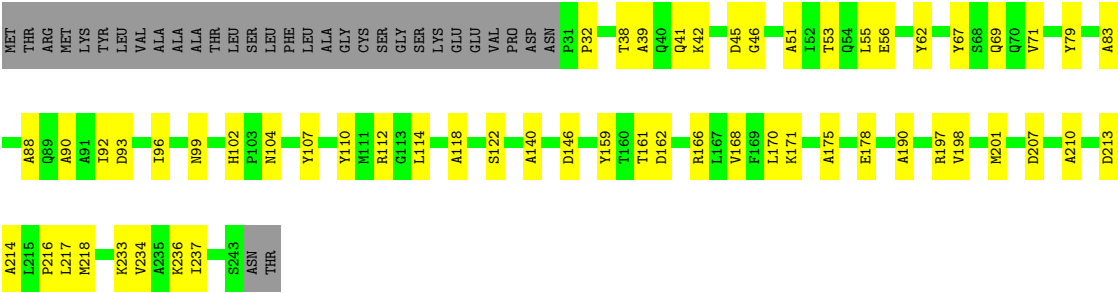


- Molecule 1: Outer membrane protein assembly factor BamA

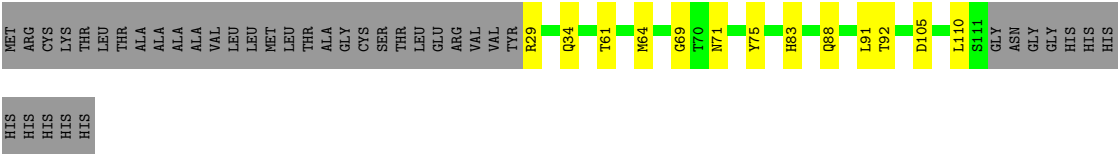




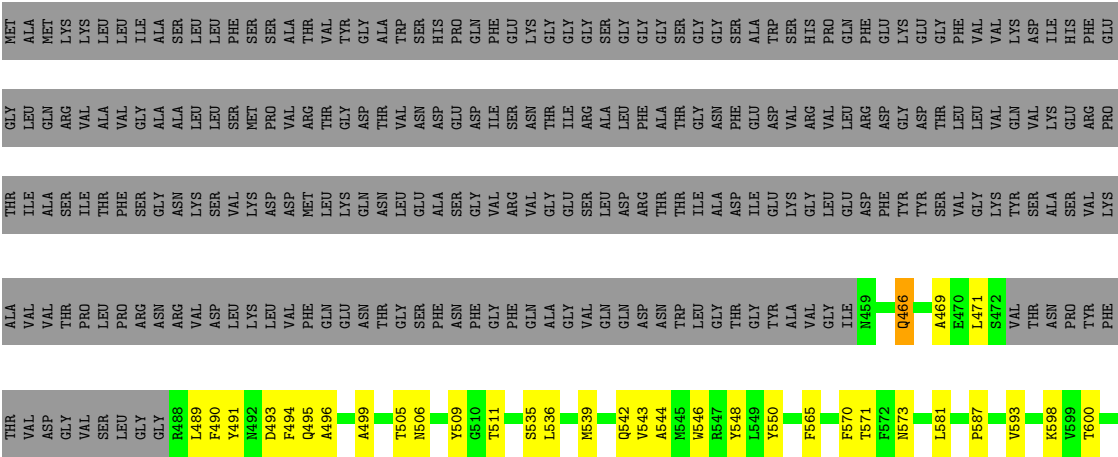
● Molecule 4: Outer membrane protein assembly factor BamD

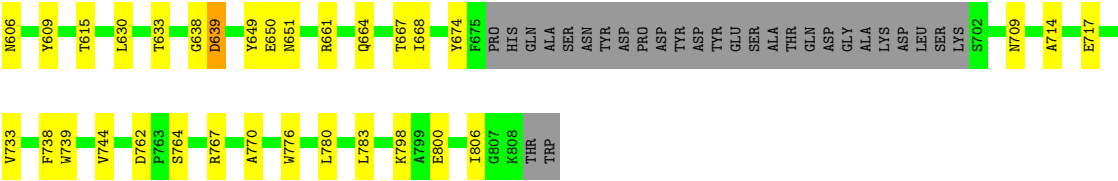


● Molecule 5: Outer membrane protein assembly factor BamE



● Molecule 6: Outer membrane protein assembly factor BamA,Outer membrane protein assembly factor BamA,Outer membrane protein assembly factor BamA,Outer membrane protein assembly factor BamA







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	223353	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	70	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	58717	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 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	0.26	0/5548	0.43	0/7462
2	B	0.24	0/2564	0.46	0/3495
3	C	0.29	0/929	0.54	0/1213
4	D	0.26	0/1761	0.44	0/2390
5	E	0.24	0/659	0.45	0/899
6	F	0.25	0/2543	0.47	0/3457
All	All	0.26	0/14004	0.45	0/18916

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	2
2	B	0	1
4	D	0	1
6	F	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	644	LYS	Peptide
1	A	645	GLU	Peptide
2	B	221	MET	Peptide
4	D	83	ALA	Peptide
6	F	466	GLN	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	5429	0	4735	62	0
2	B	2522	0	2459	47	0
3	C	919	0	570	56	0
4	D	1722	0	1668	67	0
5	E	645	0	625	11	0
6	F	2468	0	2255	38	0
All	All	13705	0	12312	239	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 9.

The worst 5 of 239 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)
3:C:53:PRO:HG3	4:D:237:ILE:HB	1.39	1.02
3:C:56:MET:SD	4:D:233:LYS:HB3	2.00	1.02
1:A:246:SER:HG	2:B:195:ARG:N	1.59	1.00
3:C:56:MET:HE1	4:D:236:LYS:HB2	1.52	0.92
4:D:45:ASP:OD1	4:D:46:GLY:N	2.05	0.89

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 PDB entries followed by that with respect to all EM entries.

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	752/810 (93%)	730 (97%)	22 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	330/392 (84%)	317 (96%)	13 (4%)	0	100	100
3	C	179/344 (52%)	166 (93%)	12 (7%)	1 (1%)	27	68
4	D	211/245 (86%)	202 (96%)	9 (4%)	0	100	100
5	E	81/123 (66%)	78 (96%)	3 (4%)	0	100	100
6	F	303/578 (52%)	295 (97%)	8 (3%)	0	100	100
All	All	1856/2492 (74%)	1788 (96%)	67 (4%)	1 (0%)	56	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	64	ASP

### 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 PDB entries followed by that with respect to all EM entries.

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	519/688 (75%)	519 (100%)	0	100	100
2	B	264/321 (82%)	263 (100%)	1 (0%)	92	95
3	C	44/276 (16%)	41 (93%)	3 (7%)	17	50
4	D	178/204 (87%)	178 (100%)	0	100	100
5	E	72/103 (70%)	72 (100%)	0	100	100
6	F	263/482 (55%)	261 (99%)	2 (1%)	83	91
All	All	1340/2074 (65%)	1334 (100%)	6 (0%)	92	95

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	64	ASP
6	F	767	ARG
3	C	87	GLN
3	C	50	LEU
6	F	639	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	302	ASN
4	D	60	ASN
6	F	765	ASN
2	B	324	HIS
2	B	334	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](#)

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.