WORLDWIDE PDB
PROTEIN DATA BANK

EMDataBank
Unified Data Resource for 3DEM

wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 23, 2017 – 07:49 PM EDT

PDB ID	:	5LJO
EMDB ID:	:	EMD-4061
Title	:	E. coli BAM complex (BamABCDE) by cryoEM
Authors	:	Iadanza, M.G.; Ranson, N.A.; Radford, S.E.; Higgins, A.J.; Schffrin, B.; Calabrese, A.N.; Ashcroft, A.E.; Brockwell, D.J.
Deposited on	:	unknown
Resolution	:	4.90 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
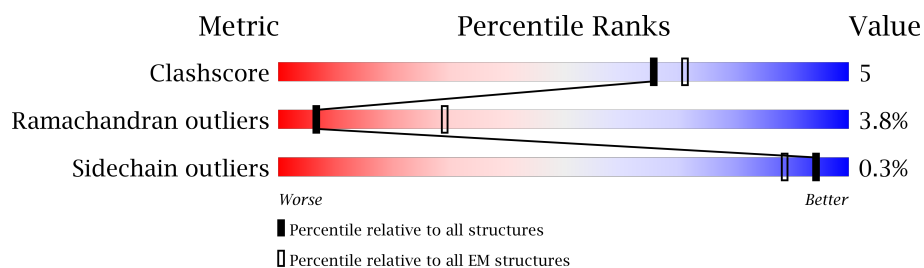with specific help available everywhere you see the ⓘ symbol.

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 4.90 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		3.8%
Sidechain outliers		0.3%

Worse *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 <=5%

Mol	Chain	Length	Quality of chain
1	B	371	86% 12% •
2	C	165	91% 7% •
3	D	218	93% 7%
4	E	87	87% 10% •
5	A	783	88% 10% •

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 24947 atoms, of which 12255 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 BamB.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	371	Total 5534	C 1754	H 2739	N 478	O 557	S 6	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	165	Total 2498	C 784	H 1241	N 223	O 248	S 2	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	218	Total 3461	C 1109	H 1700	N 309	O 336	S 7	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	87	Total 1352	C 432	H 667	N 119	O 132	S 2	0	0

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

| Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	783	Total 12102	C 3907	H 5908	N 1043	O 1228	S 16	0	0

3 Residue-property plots ⓘ

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. 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. Stretches of 2 or more consecutive
residues without any outlier are shown as a green connector. Residues present in the sample, but
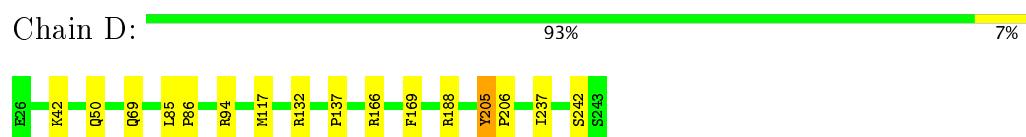not in the model, are shown in grey.

- Molecule 1: Outer membrane protein assembly factor BamB
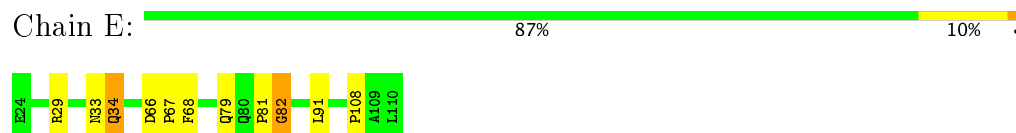
Chain B:
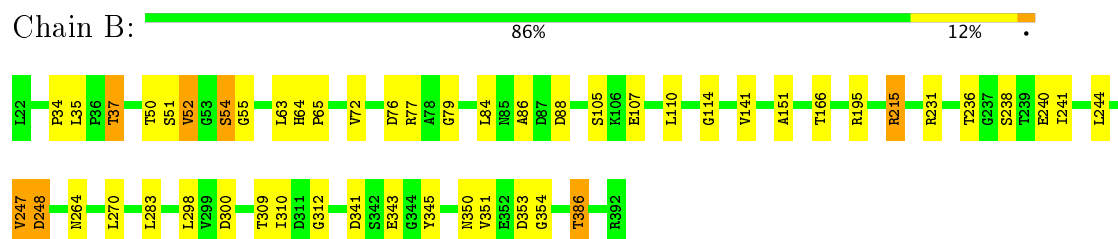
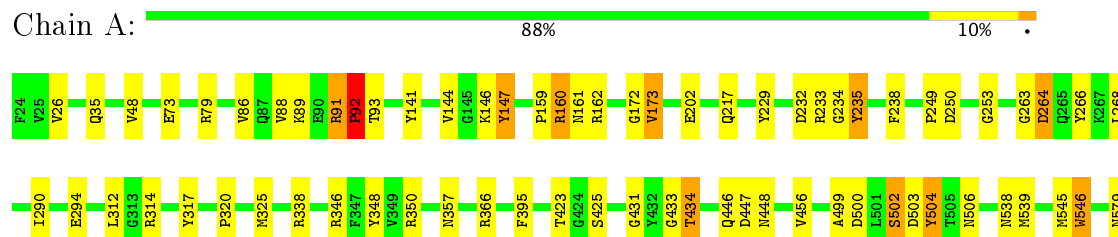- Molecule 2: Outer membrane protein assembly factor BamC
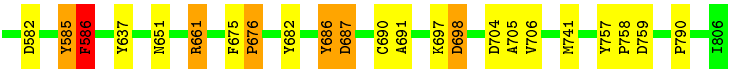
Chain C:
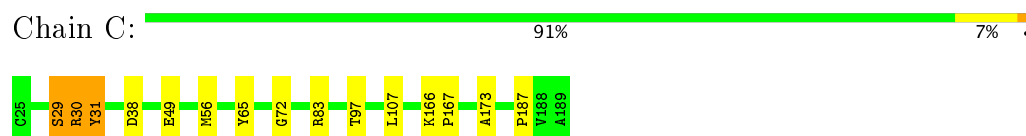
- Molecule 3: Outer membrane protein assembly factor BamD

Chain D:

- Molecule 4: Outer membrane protein assembly factor BamE

Chain E:

- Molecule 5: Outer membrane protein assembly factor BamA

Chain A:

4   Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	95878	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 $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k 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	#$|Z|$ >2	RMSZ	#$|Z|$ >2
1	B	0.79	0/2846	0.82	3/3881 (0.1%)
2	C	0.69	0/1281	0.77	0/1748
3	D	0.78	0/1801	0.81	5/2447 (0.2%)
4	E	0.72	0/700	0.81	0/955
5	A	0.80	0/6337	0.83	9/8598 (0.1%)
All	All	0.78	0/12965	0.82	17/17629 (0.1%)

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	B	0	4
2	C	0	2
5	A	0	4
All	All	0	10

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	348	TYR	CB-CG-CD1	-9.73	115.16	121.00
1	B	195	ARG	NE-CZ-NH2	-8.33	116.14	120.30
5	A	366	ARG	NE-CZ-NH2	-6.33	117.13	120.30
5	A	346	ARG	NE-CZ-NH1	6.03	123.32	120.30
3	D	166	ARG	NE-CZ-NH2	-5.64	117.48	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	431	GLY	Mainchain
5	A	92	PRO	Mainchain,Peptide
1	B	353	ASP	Mainchain,Peptide
1	B	54	SER	Mainchain,Peptide
2	C	72	GLY	Mainchain,Peptide

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	B	2795	2739	2738	31	0
2	C	1257	1241	1240	13	0
3	D	1761	1700	1699	8	0
4	E	685	667	666	8	0
5	A	6194	5908	5907	57	0
All	All	12692	12255	12250	116	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 5.

The worst 5 of 116 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:B:50:THR:O	1:B:50:THR:HG23	1.56	1.04
3:D:169:PHE:CD1	3:D:169:PHE:O	2.33	0.81
5:A:586:PHE:CD2	5:A:586:PHE:O	2.37	0.77
1:B:50:THR:O	1:B:50:THR:CG2	2.31	0.77
5:A:586:PHE:CD2	5:A:586:PHE:C	2.64	0.69

There are no symmetry-related clashes.

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 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	B	369/371 (100%)	313 (85%)	39 (11%)	17 (5%)	3	29
2	C	163/165 (99%)	138 (85%)	19 (12%)	6 (4%)	4	34
3	D	216/218 (99%)	208 (96%)	5 (2%)	3 (1%)	13	54
4	E	85/87 (98%)	68 (80%)	12 (14%)	5 (6%)	2	23
5	A	781/783 (100%)	674 (86%)	76 (10%)	31 (4%)	3	32
All	All	1614/1624 (99%)	1401 (87%)	151 (9%)	62 (4%)	7	33

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	PRO
1	B	247	VAL
1	B	386	THR
2	C	30	ARG
2	C	31	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 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	B	302/302 (100%)	302 (100%)	0	100	100
2	C	133/133 (100%)	133 (100%)	0	100	100
3	D	183/183 (100%)	183 (100%)	0	100	100
4	E	76/76 (100%)	76 (100%)	0	100	100
5	A	668/668 (100%)	664 (99%)	4 (1%)	89	94
All	All	1362/1362 (100%)	1358 (100%)	4 (0%)	94	96

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

Mol	Chain	Res	Type
5	A	79	ARG
5	A	546	TRP
5	A	586	PHE
5	A	661	ARG

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

Mol	Chain	Res	Type
1	B	302	ASN
4	E	89	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 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.