



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 19, 2016 – 11:07 PM EDT

PDB ID : 5D0Q
Title : BamACDE complex, outer membrane beta-barrel assembly machinery (BAM) complex
Authors : Gu, Y.; Paterson, N.; Zeng, Y.; Dong, H.; Wang, W.; Dong, C.
Deposited on : 2015-08-03
Resolution : 3.50 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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

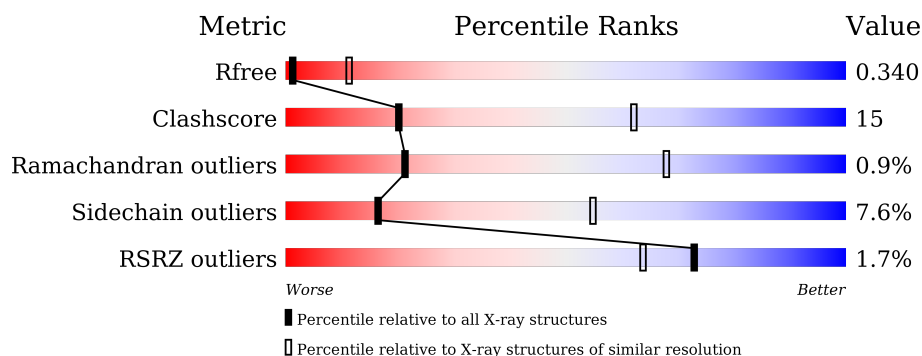
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



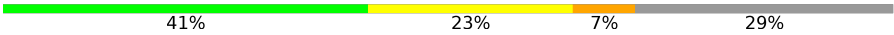
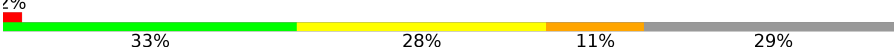
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	810	<div> <div></div> <div> <div></div> <div>65%</div> <div>26%</div> <div>• 6%</div> </div> </div>
1	F	810	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>• 6%</div> </div> </div>
2	C	344	<div> <div></div> <div> <div></div> <div>60%</div> <div>29%</div> <div>• 8%</div> </div> </div>
2	G	344	<div> <div></div> <div> <div>17%</div> <div>7%</div> <div>•</div> <div>75%</div> </div> </div>
3	D	245	<div> <div></div> <div> <div></div> <div>64%</div> <div>24%</div> <div>• 11%</div> </div> </div>
3	H	245	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>25%</div> <div>• 11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	E	123	 41% 23% 7% 29%
4	I	123	 2% 33% 28% 11% 29%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19905 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	762	Total	C	N	O	S	Se	0	0	0
			6006	3786	1009	1195	2	14			
1	F	761	Total	C	N	O	S	Se	0	1	0
			5998	3781	1008	1193	2	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP P0A940
F	1	MSE	-	initiating methionine	UNP P0A940

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	316	Total	C	N	O	S	Se	0	0	0
			2386	1478	421	479	1	7			
2	G	86	Total	C	N	O	Se		0	0	0
			623	386	107	126	4				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	-	initiating methionine	UNP P0A903
G	1	MSE	-	initiating methionine	UNP P0A903

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	218	Total	C	N	O	Se		0	0	0
			1761	1109	309	336	7				
3	H	218	Total	C	N	O	Se		0	0	0
			1761	1109	309	336	7				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	-	initiating methionine	UNP P0AC02
H	1	MSE	-	initiating methionine	UNP P0AC02

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	87	Total	C	N	O	Se	0	0	0
			685	432	119	132	2			
4	I	87	Total	C	N	O	Se	0	0	0
			685	432	119	132	2			

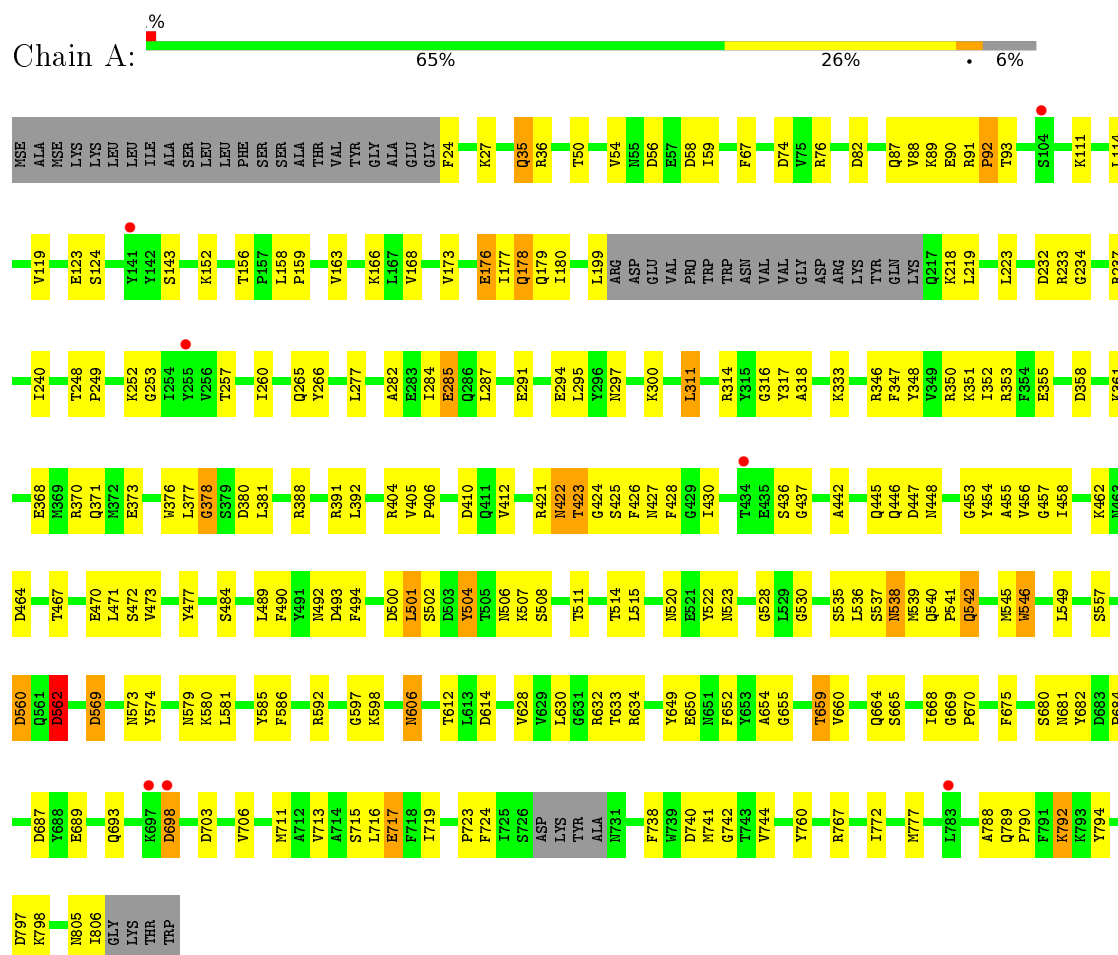
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MSE	-	initiating methionine	UNP P0A937
E	114	GLY	-	expression tag	UNP P0A937
E	115	GLY	-	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
E	120	HIS	-	expression tag	UNP P0A937
E	121	HIS	-	expression tag	UNP P0A937
E	122	HIS	-	expression tag	UNP P0A937
E	123	HIS	-	expression tag	UNP P0A937
I	1	MSE	-	initiating methionine	UNP P0A937
I	114	GLY	-	expression tag	UNP P0A937
I	115	GLY	-	expression tag	UNP P0A937
I	116	HIS	-	expression tag	UNP P0A937
I	117	HIS	-	expression tag	UNP P0A937
I	118	HIS	-	expression tag	UNP P0A937
I	119	HIS	-	expression tag	UNP P0A937
I	120	HIS	-	expression tag	UNP P0A937
I	121	HIS	-	expression tag	UNP P0A937
I	122	HIS	-	expression tag	UNP P0A937
I	123	HIS	-	expression tag	UNP P0A937

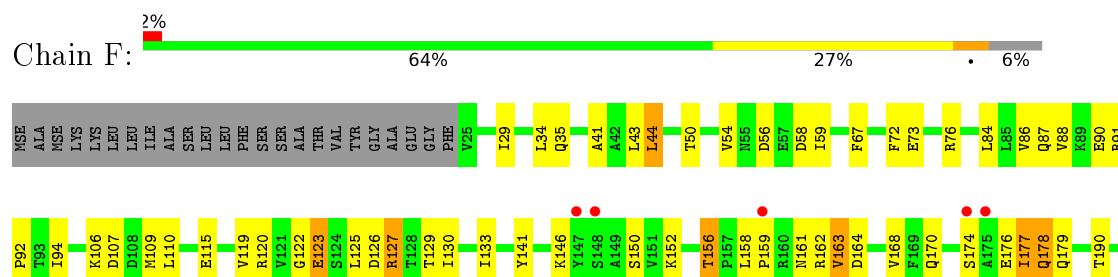
3 Residue-property plots

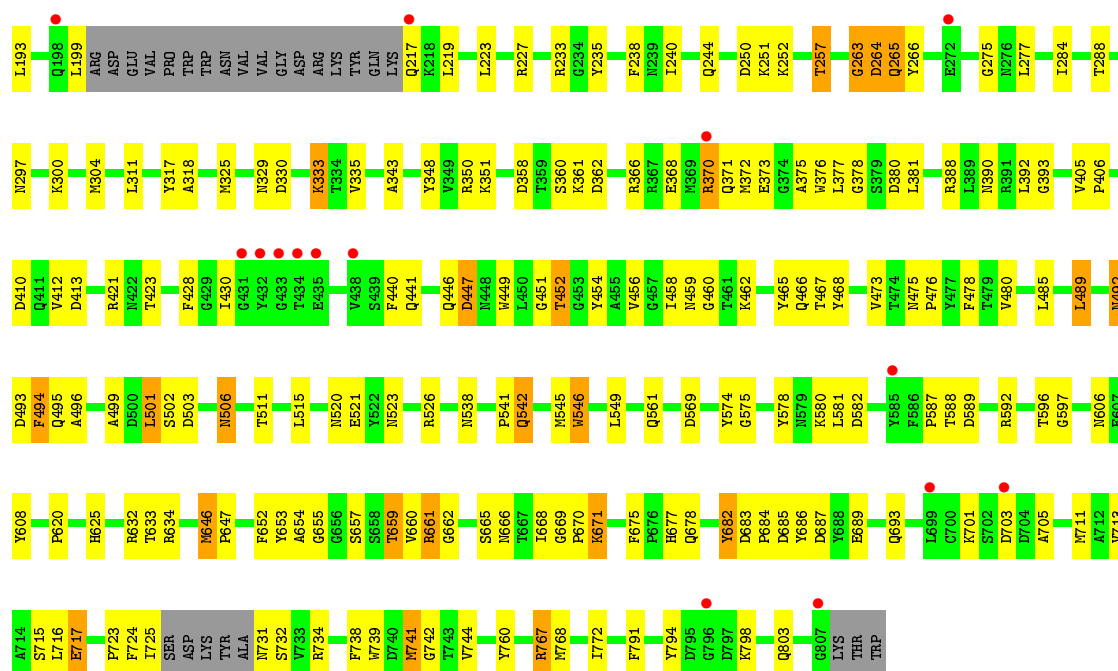
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Outer membrane protein assembly factor BamA

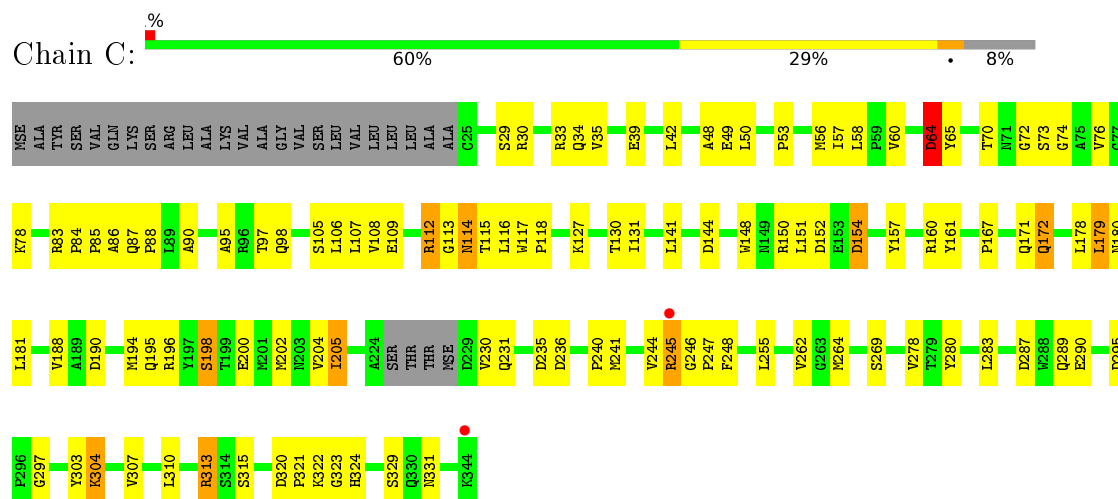


- Molecule 1: Outer membrane protein assembly factor BamA

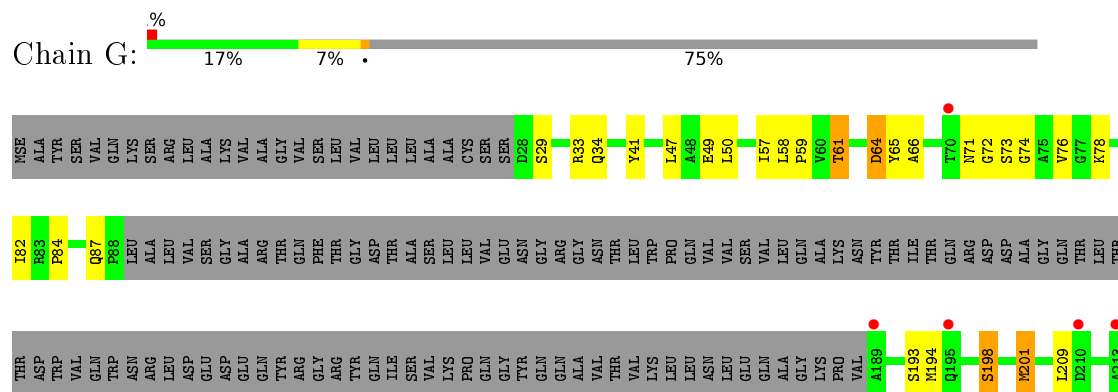


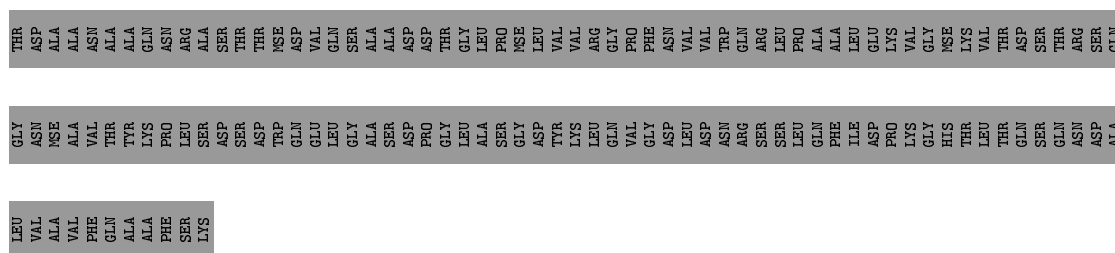


• Molecule 2: Outer membrane protein assembly factor BamC

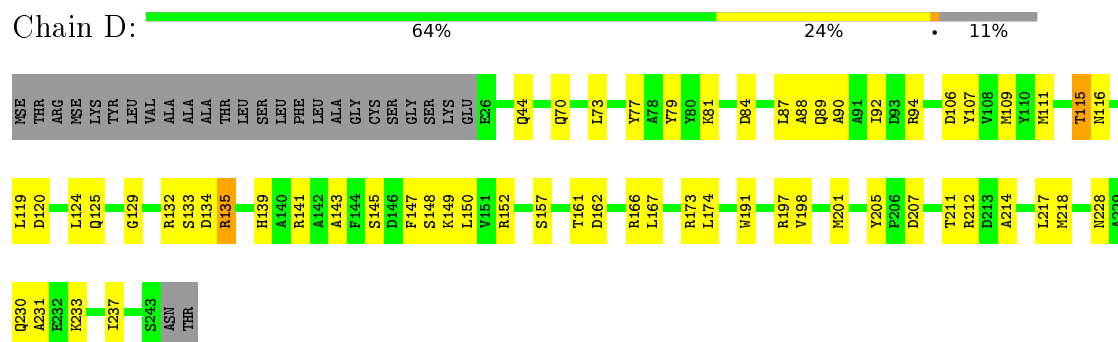


• Molecule 2: Outer membrane protein assembly factor BamC

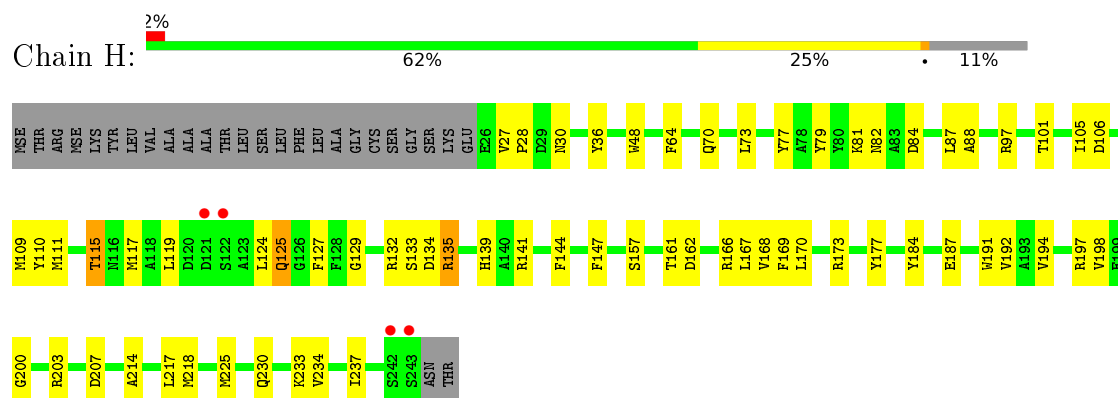




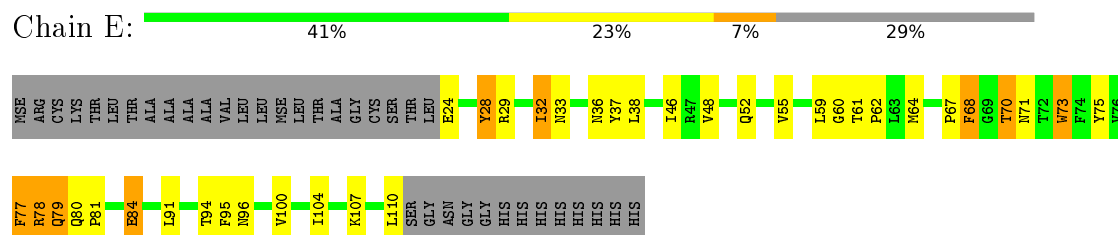
- Molecule 3: Outer membrane protein assembly factor BamD



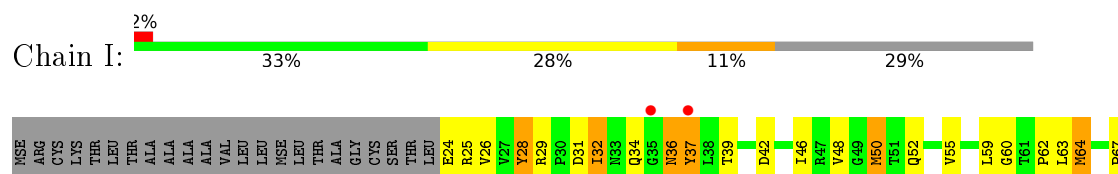
- Molecule 3: Outer membrane protein assembly factor BamD



- Molecule 4: Outer membrane protein assembly factor BamE



- Molecule 4: Outer membrane protein assembly factor BamE





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	254.16Å 254.16Å 179.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 3.50 29.94 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.94-3.50) 100.0 (29.94-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.47Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.314 , 0.340 0.315 , 0.340	Depositor DCC
R_{free} test set	3724 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	128.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 30.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	3 of 74050 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19905	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.32	0/6126	0.59	2/8285 (0.0%)
1	F	0.33	0/6120	0.60	3/8277 (0.0%)
2	C	0.28	0/2420	0.55	0/3281
2	G	0.27	0/629	0.52	0/846
3	D	0.30	0/1794	0.56	0/2426
3	H	0.31	0/1794	0.56	0/2426
4	E	0.35	0/698	0.72	0/949
4	I	0.40	0/698	0.75	0/949
All	All	0.32	0/20279	0.59	5/27439 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	661	ARG	NE-CZ-NH1	-8.13	116.24	120.30
1	A	378	GLY	N-CA-C	-6.02	98.05	113.10
1	F	44	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	501	LEU	CA-CB-CG	5.43	127.80	115.30
1	F	263	GLY	N-CA-C	-5.21	100.08	113.10

There are no chirality outliers.

There are no planarity outliers.

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	6006	0	5728	165	0
1	F	5998	0	5728	169	0
2	C	2386	0	2336	84	0
2	G	623	0	612	19	0
3	D	1761	0	1699	50	0
3	H	1761	0	1699	57	0
4	E	685	0	666	44	0
4	I	685	0	666	48	0
All	All	19905	0	19134	573	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 15.

The worst 5 of 573 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:240:ILE:HA	1:A:260:ILE:HG22	1.53	0.90
1:A:632:ARG:HB2	1:A:715:SER:HB3	1.58	0.86
1:F:91:ARG:HD3	1:F:127:ARG:H	1.41	0.85
2:C:116:LEU:HB3	2:C:172:GLN:HE22	1.42	0.84
1:F:561:GLN:HB3	1:F:677:HIS:HE1	1.44	0.82

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 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	756/810 (93%)	688 (91%)	62 (8%)	6 (1%)	24 70
1	F	756/810 (93%)	696 (92%)	57 (8%)	3 (0%)	39 81
2	C	312/344 (91%)	288 (92%)	21 (7%)	3 (1%)	19 66
2	G	82/344 (24%)	70 (85%)	10 (12%)	2 (2%)	7 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	216/245 (88%)	209 (97%)	7 (3%)	0	100	100
3	H	216/245 (88%)	209 (97%)	7 (3%)	0	100	100
4	E	85/123 (69%)	78 (92%)	4 (5%)	3 (4%)	4	38
4	I	85/123 (69%)	76 (89%)	4 (5%)	5 (6%)	2	22
All	All	2508/3044 (82%)	2314 (92%)	172 (7%)	22 (1%)	21	68

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	36	ASN
4	E	70	THR
2	C	329	SER
1	F	178	GLN
1	F	502	SER

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	649/672 (97%)	600 (92%)	49 (8%)	16	55
1	F	648/672 (96%)	596 (92%)	52 (8%)	15	52
2	C	254/267 (95%)	232 (91%)	22 (9%)	13	48
2	G	63/267 (24%)	56 (89%)	7 (11%)	8	35
3	D	183/195 (94%)	180 (98%)	3 (2%)	70	89
3	H	183/195 (94%)	178 (97%)	5 (3%)	52	83
4	E	76/99 (77%)	65 (86%)	11 (14%)	4	23
4	I	76/99 (77%)	64 (84%)	12 (16%)	3	19
All	All	2132/2466 (86%)	1971 (92%)	161 (8%)	16	55

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	124	LEU
1	F	67	PHE
4	I	68	PHE
4	E	32	ILE
4	E	79	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	230	GLN
4	E	79	GLN
4	I	80	GLN
3	D	138	GLN
3	D	139	HIS

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.

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	748/810 (92%)	-0.25	7 (0%) 85 78	100, 156, 213, 238	0
1	F	747/810 (92%)	-0.20	20 (2%) 58 47	116, 158, 215, 243	3 (0%)
2	C	309/344 (89%)	-0.24	2 (0%) 90 85	95, 137, 202, 206	0
2	G	82/344 (23%)	0.11	5 (6%) 25 19	137, 161, 271, 279	0
3	D	211/245 (86%)	-0.24	0 100 100	87, 109, 138, 154	0
3	H	211/245 (86%)	0.02	4 (1%) 70 60	126, 147, 194, 202	0
4	E	85/123 (69%)	-0.37	0 100 100	121, 141, 168, 178	0
4	I	85/123 (69%)	-0.02	3 (3%) 48 38	131, 151, 174, 196	0
All	All	2478/3044 (81%)	-0.20	41 (1%) 73 64	87, 150, 207, 279	3 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	243	SER	8.9
1	F	432	TYR	5.4
1	F	198	GLN	4.9
1	F	175	ALA	4.1
1	F	217	GLN	4.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.