



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:37 AM GMT

PDB ID : 4K3C  
Title : The crystal structure of BamA from Haemophilus ducreyi lacking POTRA domains 1-3  
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Deposited on : 2013-04-10  
Resolution : 2.91 Å(reported)

This is a full wwPDB validation 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 <http://wwpdb.org/ValidationPDFNotes.html>

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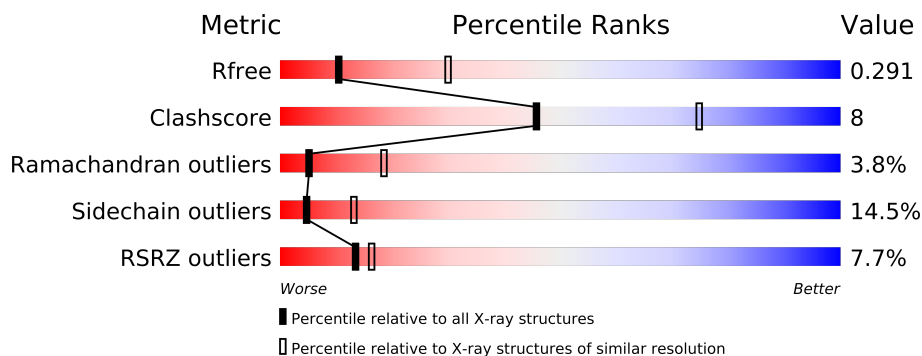
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.91 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))
$R_{free}$	66092	1172 (2.94-2.90)
Clashscore	79885	1461 (2.94-2.90)
Ramachandran outliers	78287	1419 (2.94-2.90)
Sidechain outliers	78261	1421 (2.94-2.90)
RSRZ outliers	66119	1173 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	532	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3959 atoms, of which 0 are hydrogen and 0 are deuterium.

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	532	Total	C	N	O	S	0	0	0
			3947	2484	686	770	7			

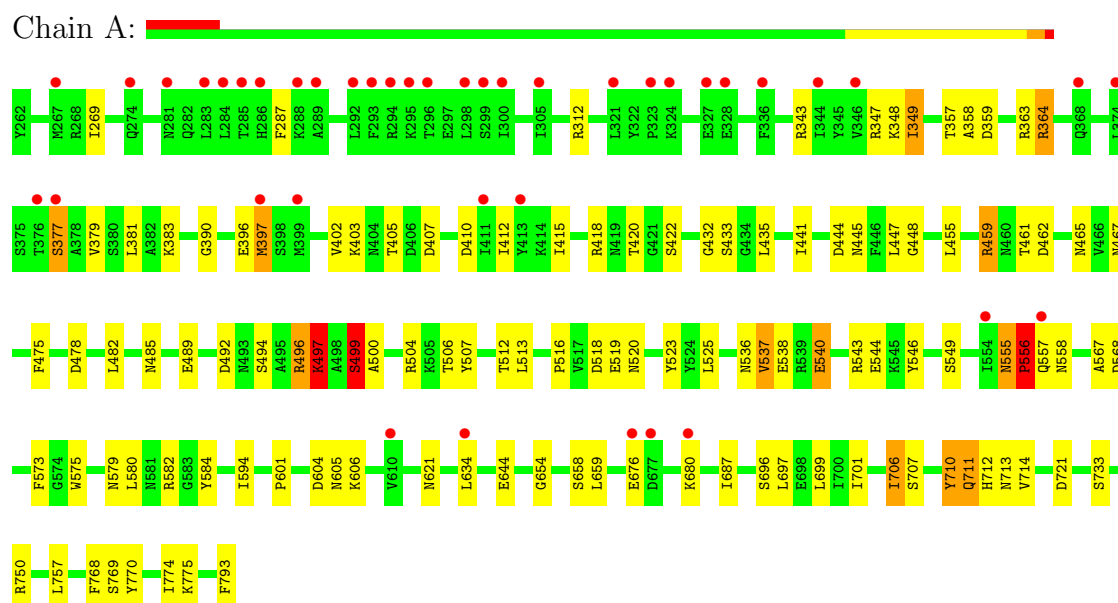
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		

### 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.78Å 88.16Å 244.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.91 46.89 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.95-2.91) 95.8 (46.89-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1042)	Depositor
R, $R_{free}$	0.220 , 0.270 0.247 , 0.291	Depositor DCC
$R_{free}$ test set	1958 reflections (9.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.4	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 47.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 23388 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	3959	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.51	0/4034	0.71	3/5470 (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	A	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	500	ALA	N-CA-C	-5.70	95.60	111.00
1	A	432	GLY	N-CA-C	-5.19	100.12	113.10
1	A	567	ALA	C-N-CA	5.04	134.29	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	497	LYS	Peptide
1	A	499	SER	Peptide
1	A	556	PRO	Peptide

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3947	0	8	33	0
2	A	12	0	0	0	0
All	All	3959	0	8	33	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (33) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:379:VAL:CG1	1:A:397:MET:CE	2.56	0.84
1:A:347:ARG:NH2	1:A:410:ASP:OD2	2.23	0.72
1:A:555:ASN:O	1:A:556:PRO:O	2.09	0.68
1:A:462:ASP:OD2	1:A:496:ARG:NH1	2.26	0.68
1:A:390:GLY:O	1:A:418:ARG:NE	2.28	0.66
1:A:555:ASN:C	1:A:556:PRO:O	2.36	0.63
1:A:540:GLU:OE1	1:A:543:ARG:N	2.35	0.60
1:A:445:ASN:O	1:A:448:GLY:N	2.35	0.60
1:A:359:ASP:OD1	1:A:363:ARG:NH2	2.34	0.60
1:A:489:GLU:OE2	1:A:504:ARG:NH1	2.37	0.57
1:A:467:ASN:OD1	1:A:485:ASN:ND2	2.39	0.55
1:A:497:LYS:C	1:A:499:SER:N	2.61	0.54
1:A:696:SER:OG	1:A:721:ASP:OD1	2.26	0.53
1:A:402:VAL:O	1:A:405:THR:OG1	2.27	0.52
1:A:710:TYR:O	1:A:712:HIS:O	2.27	0.52
1:A:706:ILE:O	1:A:707:SER:OG	2.30	0.49
1:A:523:TYR:CE1	1:A:575:TRP:CD1	3.01	0.49
1:A:604:ASP:O	1:A:606:LYS:N	2.45	0.49
1:A:435:LEU:O	1:A:459:ARG:NH1	2.46	0.48
1:A:555:ASN:O	1:A:556:PRO:C	2.51	0.47
1:A:757:LEU:O	1:A:768:PHE:N	2.47	0.47
1:A:349:ILE:O	1:A:363:ARG:NH1	2.49	0.46
1:A:377:SER:O	1:A:381:LEU:N	2.49	0.45
1:A:518:ASP:O	1:A:520:ASN:N	2.51	0.44
1:A:556:PRO:C	1:A:558:ASN:N	2.71	0.44
1:A:546:TYR:OH	1:A:605:ASN:OD1	2.36	0.43
1:A:513:LEU:N	1:A:525:LEU:O	2.51	0.43
1:A:492:ASP:OD1	1:A:494:SER:OG	2.37	0.42
1:A:654:GLY:N	1:A:658:SER:OG	2.52	0.41
1:A:707:SER:CB	1:A:711:GLN:NE2	2.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:536:ASN:OD1	1:A:537:VAL:N	2.53	0.41
1:A:582:ARG:NH1	1:A:584:TYR:O	2.54	0.41
1:A:712:HIS:O	1:A:713:ASN:CB	2.69	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	530/532 (100%)	459 (87%)	51 (10%)	20 (4%)	<b>5</b> <b>18</b>

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	PHE
1	A	357	THR
1	A	497	LYS
1	A	556	PRO
1	A	557	GLN
1	A	568	ASP
1	A	676	GLU
1	A	358	ALA
1	A	433	SER
1	A	475	PHE
1	A	496	ARG
1	A	580	LEU
1	A	706	ILE
1	A	269	ILE
1	A	499	SER
1	A	377	SER
1	A	364	ARG
1	A	537	VAL
1	A	555	ASN
1	A	516	PRO



### 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	379/445 (85%)	324 (86%)	55 (14%)	<b>5</b> <b>13</b>

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	ARG
1	A	343	ARG
1	A	348	LYS
1	A	349	ILE
1	A	364	ARG
1	A	383	LYS
1	A	396	GLU
1	A	397	MET
1	A	403	LYS
1	A	407	ASP
1	A	412	ILE
1	A	415	ILE
1	A	420	THR
1	A	422	SER
1	A	441	ILE
1	A	444	ASP
1	A	447	LEU
1	A	455	LEU
1	A	459	ARG
1	A	461	THR
1	A	465	ASN
1	A	478	ASP
1	A	482	LEU
1	A	497	LYS
1	A	506	THR
1	A	507	TYR
1	A	512	THR
1	A	519	GLU
1	A	538	GLU
1	A	540	GLU
1	A	544	GLU

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Mol	Chain	Res	Type
1	A	549	SER
1	A	573	PHE
1	A	579	ASN
1	A	594	ILE
1	A	601	PRO
1	A	621	ASN
1	A	634	LEU
1	A	644	GLU
1	A	659	LEU
1	A	680	LYS
1	A	687	ILE
1	A	697	LEU
1	A	699	LEU
1	A	701	ILE
1	A	710	TYR
1	A	711	GLN
1	A	714	VAL
1	A	733	SER
1	A	750	ARG
1	A	769	SER
1	A	770	TYR
1	A	774	ILE
1	A	775	LYS
1	A	793	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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, 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	532/532 (100%)	0.19	41 (7%)	13 16	30, 60, 189, 230	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ALA	8.1
1	A	285	THR	8.1
1	A	293	PHE	7.6
1	A	296	THR	7.0
1	A	292	LEU	6.5
1	A	284	LEU	5.3
1	A	328	GLU	4.5
1	A	288	LYS	4.1
1	A	374	LEU	4.0
1	A	294	ARG	4.0
1	A	286	HIS	3.8
1	A	267	MET	3.8
1	A	295	LYS	3.7
1	A	274	GLN	3.2
1	A	300	ILE	3.2
1	A	298	LEU	3.1
1	A	323	PRO	3.0
1	A	411	ILE	2.9
1	A	399	MET	2.9
1	A	676	GLU	2.9
1	A	299	SER	2.8
1	A	368	GLN	2.8
1	A	327	GLU	2.7
1	A	557	GLN	2.7
1	A	677	ASP	2.7
1	A	376	THR	2.7
1	A	554	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	283	LEU	2.4
1	A	377	SER	2.4
1	A	634	LEU	2.4
1	A	305	ILE	2.3
1	A	397	MET	2.3
1	A	610	VAL	2.3
1	A	321	LEU	2.3
1	A	344	ILE	2.2
1	A	346	VAL	2.2
1	A	281	ASN	2.2
1	A	680	LYS	2.1
1	A	324	LYS	2.0
1	A	413	TYR	2.0
1	A	336	PHE	2.0

## 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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.