



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2022 – 04:12 am BST

PDB ID : 7R1V  
Title : Crystal structure of E.coli BamA beta-barrel in complex with dynobactin A  
Authors : Jakob, R.P.; Hiller, S.; Maier, T.  
Deposited on : 2022-02-03  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.30
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

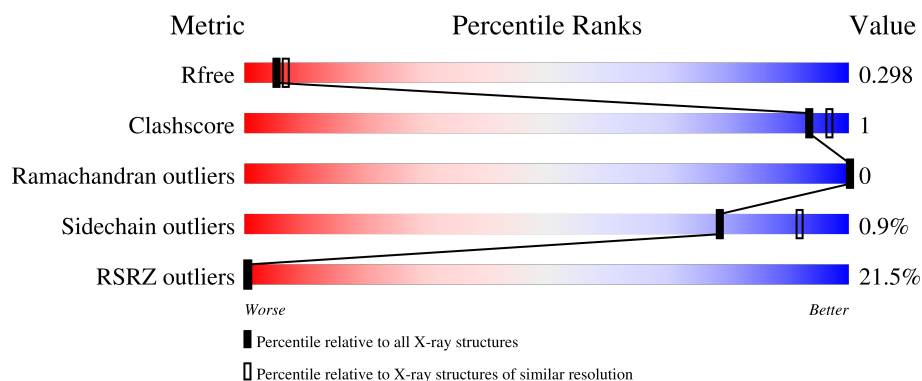
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	392	<div> <div>20%</div> <div>91%</div> <div>6%</div> </div>
2	B	10	<div> <div>10%</div> <div>80%</div> <div>20%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5770 atoms, of which 2707 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	367	Total	C	H	N	O	S	0	0	0
			5524	1842	2632	466	576	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	HIS	-	expression tag	UNP P0A942
A	420	MET	-	expression tag	UNP P0A942
A	690	SER	CYS	engineered mutation	UNP P0A942
A	700	SER	CYS	engineered mutation	UNP P0A942

- Molecule 2 is a protein called Dynobactin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	10	Total	C	H	N	O	0	0	0
			169	60	75	18	16			

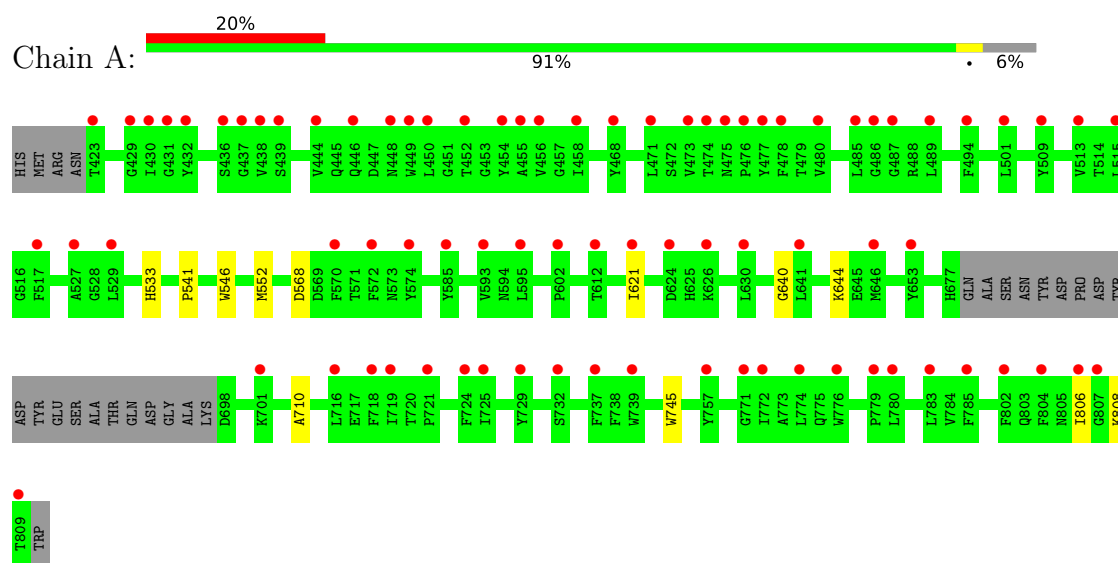
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		
3	B	7	Total	O	0	0
			7	7		

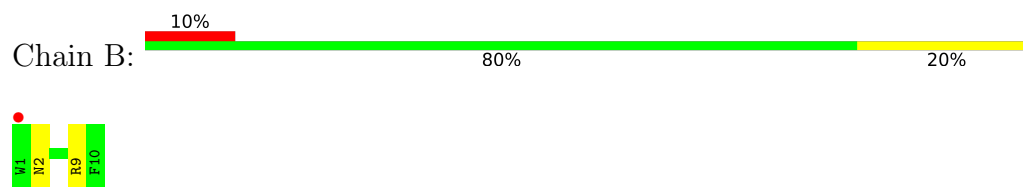
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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 2: Dynobactin A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.79Å 71.32Å 116.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 2.50 48.36 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.36-2.50) 99.7 (48.36-2.50)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.3 (18-SEP-2020)	Depositor
R, $R_{free}$	0.246 , 0.275 0.253 , 0.298	Depositor DCC
$R_{free}$ test set	985 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtriage
Anisotropy	0.957	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5770	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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	0.44	0/2980	0.63	0/4056
2	B	0.40	0/98	0.64	0/131
All	All	0.44	0/3078	0.63	0/4187

There are no bond length outliers.

There are no bond angle outliers.

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	2892	2632	2648	8	0
2	B	94	75	81	1	0
3	A	70	0	0	1	0
3	B	7	0	0	0	0
All	All	3063	2707	2729	8	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 1.

All (8) 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:808:LYS:HD2	2:B:2:ASN:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:MET:SD	1:A:644:LYS:HD2	2.43	0.59
1:A:533:HIS:HD2	1:A:568:ASP:OD1	1.92	0.52
1:A:621:ILE:O	1:A:621:ILE:CG1	2.57	0.51
1:A:710:ALA:CB	1:A:745:TRP:CE2	2.98	0.47
1:A:710:ALA:HB1	1:A:745:TRP:CE2	2.52	0.43
1:A:541:PRO:HG2	3:A:936:HOH:O	2.19	0.43
1:A:640:GLY:HA3	1:A:644:LYS:O	2.19	0.42

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	363/392 (93%)	346 (95%)	17 (5%)	0	100	100
2	B	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	371/402 (92%)	353 (95%)	18 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	307/328 (94%)	305 (99%)	2 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	10/10 (100%)	9 (90%)	1 (10%)	7	15
All	All	317/338 (94%)	314 (99%)	3 (1%)	78	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	546	TRP
1	A	806	ILE
2	B	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	533	HIS
1	A	563	ASN
1	A	666	ASN
1	A	805	ASN
2	B	2	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 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

### 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	367/392 (93%)	1.23	80 (21%) <b>0</b> <b>0</b>	71, 96, 135, 163	0
2	B	10/10 (100%)	0.81	1 (10%) <b>7</b> <b>6</b>	71, 77, 91, 98	0
All	All	377/402 (93%)	1.21	81 (21%) <b>0</b> <b>0</b>	71, 95, 135, 163	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	TRP	11.7
1	A	757	TYR	8.3
1	A	718	PHE	7.6
1	A	450	LEU	7.0
1	A	476	PRO	6.7
1	A	574	TYR	6.6
1	A	739	TRP	6.2
1	A	802	PHE	6.1
1	A	485	LEU	5.5
1	A	515	LEU	5.3
1	A	456	VAL	5.3
1	A	474	THR	5.0
1	A	517	PHE	5.0
1	A	452	THR	5.0
1	A	475	ASN	4.9
1	A	804	PHE	4.9
1	A	780	LEU	4.8
1	A	724	PHE	4.6
1	A	477	TYR	4.4
1	A	486	GLY	4.4
1	A	809	THR	4.4
1	A	478	PHE	4.4
1	A	468	TYR	4.3
1	A	454	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	729	TYR	3.9
1	A	455	ALA	3.8
1	A	641	LEU	3.7
1	A	721	PRO	3.7
1	A	513	VAL	3.6
1	A	719	ILE	3.4
1	A	725	ILE	3.4
1	A	624	ASP	3.4
1	A	473	VAL	3.4
1	A	527	ALA	3.4
1	A	701	LYS	3.4
1	A	774	LEU	3.3
1	A	779	PRO	3.3
1	A	431	GLY	3.3
1	A	446	GLN	3.2
1	A	785	PHE	3.2
1	A	430	ILE	3.1
1	A	487	GLY	3.1
1	A	489	LEU	3.0
1	A	772	ILE	3.0
1	A	448	ASN	2.8
1	A	423	THR	2.7
1	A	783	LEU	2.7
1	A	593	VAL	2.6
1	A	626	LYS	2.6
1	A	572	PHE	2.6
1	A	737	PHE	2.6
1	A	595	LEU	2.6
1	A	529	LEU	2.6
1	A	621	ILE	2.6
1	A	480	VAL	2.6
1	A	612	THR	2.6
1	A	806	ILE	2.5
1	A	602	PRO	2.5
1	A	716	LEU	2.5
1	A	458	ILE	2.5
1	A	630	LEU	2.4
1	A	439	SER	2.4
1	A	509	TYR	2.4
1	A	771	GLY	2.4
1	A	432	TYR	2.4
1	A	646	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	776	TRP	2.3
2	B	1	TRP	2.3
1	A	732	SER	2.3
1	A	807	GLY	2.3
1	A	570	PHE	2.3
1	A	437	GLY	2.2
1	A	471	LEU	2.2
1	A	429	GLY	2.2
1	A	585	TYR	2.1
1	A	444	VAL	2.1
1	A	436	SER	2.1
1	A	494	PHE	2.1
1	A	653	TYR	2.0
1	A	501	LEU	2.0
1	A	438	VAL	2.0

## 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.