Full wwPDB X-ray Structure Validation Report ⓘ

Apr 3, 2023 – 01:15 pm BST

PDB ID	:	8ARV
Title	:	Structure of the EAL domain of BifA from Pseudomonas aeruginosa
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Deposited on	:	2022-08-17
Resolution	:	1.90 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*
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.

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

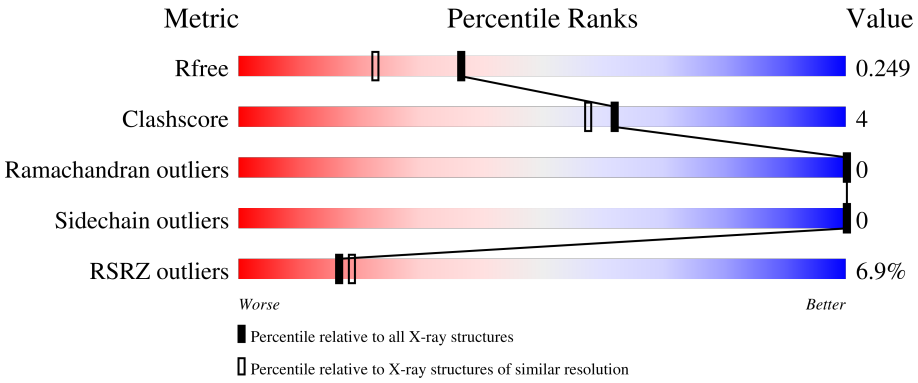
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	275	7% 83% 10% 7%
1	B	275	6% 84% 8% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4183 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 Bifunctional diguanylate cyclase/phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	9	0	0
			2040	1292	359	384	5			
1	B	254	Total	C	N	O	S	0	0	0
			2032	1286	358	383	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	404	MET	-	initiating methionine	UNP Q9HW35
A	405	GLY	-	expression tag	UNP Q9HW35
A	406	SER	-	expression tag	UNP Q9HW35
A	407	SER	-	expression tag	UNP Q9HW35
A	408	HIS	-	expression tag	UNP Q9HW35
A	409	HIS	-	expression tag	UNP Q9HW35
A	410	HIS	-	expression tag	UNP Q9HW35
A	411	HIS	-	expression tag	UNP Q9HW35
A	412	HIS	-	expression tag	UNP Q9HW35
A	413	HIS	-	expression tag	UNP Q9HW35
A	414	SER	-	expression tag	UNP Q9HW35
A	415	SER	-	expression tag	UNP Q9HW35
A	416	GLY	-	expression tag	UNP Q9HW35
A	417	LEU	-	expression tag	UNP Q9HW35
A	418	VAL	-	expression tag	UNP Q9HW35
A	419	PRO	-	expression tag	UNP Q9HW35
A	420	ARG	-	expression tag	UNP Q9HW35
A	421	GLY	-	expression tag	UNP Q9HW35
A	422	SER	-	expression tag	UNP Q9HW35
A	423	HIS	-	expression tag	UNP Q9HW35
B	404	MET	-	initiating methionine	UNP Q9HW35
B	405	GLY	-	expression tag	UNP Q9HW35
B	406	SER	-	expression tag	UNP Q9HW35
B	407	SER	-	expression tag	UNP Q9HW35
B	408	HIS	-	expression tag	UNP Q9HW35

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Chain	Residue	Modelled	Actual	Comment	Reference
B	409	HIS	-	expression tag	UNP Q9HW35
B	410	HIS	-	expression tag	UNP Q9HW35
B	411	HIS	-	expression tag	UNP Q9HW35
B	412	HIS	-	expression tag	UNP Q9HW35
B	413	HIS	-	expression tag	UNP Q9HW35
B	414	SER	-	expression tag	UNP Q9HW35
B	415	SER	-	expression tag	UNP Q9HW35
B	416	GLY	-	expression tag	UNP Q9HW35
B	417	LEU	-	expression tag	UNP Q9HW35
B	418	VAL	-	expression tag	UNP Q9HW35
B	419	PRO	-	expression tag	UNP Q9HW35
B	420	ARG	-	expression tag	UNP Q9HW35
B	421	GLY	-	expression tag	UNP Q9HW35
B	422	SER	-	expression tag	UNP Q9HW35
B	423	HIS	-	expression tag	UNP Q9HW35

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is water.

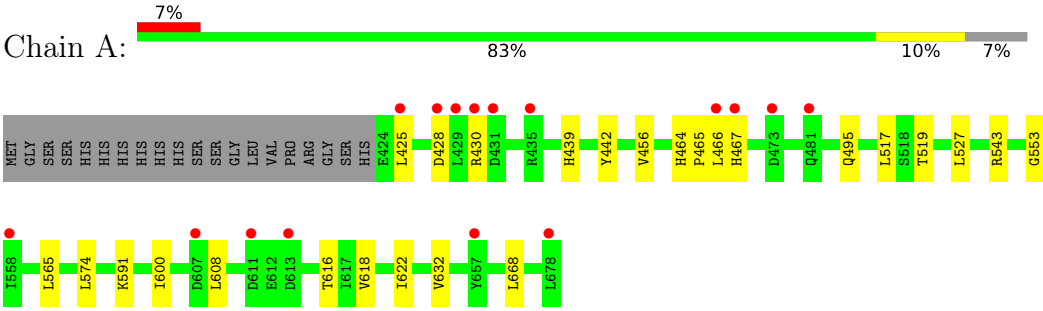
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	50	Total O 50 50	0	0
3	B	59	Total O 59 59	0	0

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.

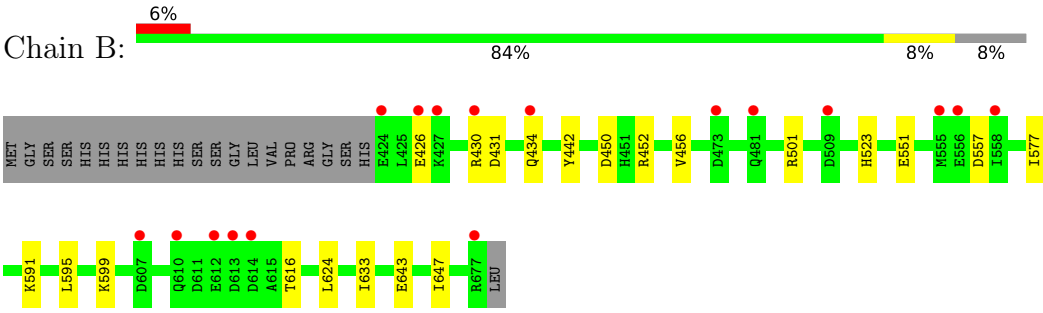
• Molecule 1: Bifunctional diguanylate cyclase/phosphodiesterase

Chain A:



• Molecule 1: Bifunctional diguanylate cyclase/phosphodiesterase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	34.70Å 117.50Å 117.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.25 – 1.90 37.25 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.25-1.90) 98.8 (37.25-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.209 , 0.249 0.209 , 0.249	Depositor DCC
R_{free} test set	1875 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.048 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4183	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.33	0/2079	0.56	0/2820
1	B	0.33	0/2071	0.55	0/2809
All	All	0.33	0/4150	0.56	0/5629

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	2040	0	2034	21	0
1	B	2032	0	2023	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	50	0	0	2	0
3	B	59	0	0	2	0
All	All	4183	0	4057	36	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 4.

All (36) 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:431:ASP:HB3	1:B:434:GLN:HE21	1.22	1.02
1:A:464:HIS:HD2	1:A:465:PRO:HD2	1.47	0.77
1:B:587:LEU:HD11	1:B:624:LEU:HD11	1.67	0.75
1:A:591:LYS:HE2	1:B:616:THR:HG21	1.68	0.75
1:A:464:HIS:CD2	1:A:465:PRO:HD2	2.22	0.75
1:A:425:LEU:HA	1:A:428:ASP:HB2	1.71	0.73
1:B:577:ILE:HD11	1:B:595:LEU:HD13	1.81	0.62
1:A:622:ILE:HD13	1:A:632:VAL:HG11	1.82	0.61
1:A:543:ARG:HG2	1:A:574:LEU:HD21	1.86	0.57
1:A:519:THR:HG23	1:A:553:GLY:HA2	1.88	0.55
1:A:616:THR:HG21	1:B:591:LYS:HE2	1.89	0.55
1:A:430:ARG:CZ	1:A:430:ARG:HB3	2.37	0.54
1:A:466:LEU:HD23	1:A:467:HIS:NE2	2.25	0.52
1:B:431:ASP:CB	1:B:434:GLN:HE21	2.09	0.50
1:A:608:LEU:HD13	1:A:618:VAL:HG21	1.94	0.49
1:B:442:TYR:HB3	1:B:456:VAL:CG1	2.43	0.49
1:A:517:LEU:HD13	1:A:527:LEU:HD21	1.95	0.48
1:A:554:LEU:HD21	1:A:565:LEU:HD11	1.96	0.47
1:B:551:GLU:OE2	1:B:585:SER:OG	2.29	0.46
1:B:501:ARG:NH2	3:B:801:HOH:O	2.34	0.45
1:A:495:GLN:NE2	3:A:802:HOH:O	2.48	0.45
1:A:464:HIS:ND1	1:A:467:HIS:ND1	2.62	0.44
1:A:442:TYR:HB3	1:A:456:VAL:CG1	2.48	0.44
1:A:600:ILE:HD11	1:A:622:ILE:HD11	2.00	0.44
1:B:643:GLU:HG2	1:B:647:ILE:CD1	2.49	0.42
1:B:551:GLU:HG3	3:B:812:HOH:O	2.18	0.42
1:A:600:ILE:HD11	1:A:622:ILE:CD1	2.49	0.42
1:B:442:TYR:HB3	1:B:456:VAL:HG11	2.01	0.42
1:B:450:ASP:OD2	1:B:452:ARG:NH2	2.53	0.42
1:B:523:HIS:CE1	1:B:557:ASP:HB3	2.54	0.42
1:B:426:GLU:OE2	1:B:430:ARG:NH2	2.52	0.41
1:A:618:VAL:O	1:A:622:ILE:HG12	2.21	0.41
1:A:442:TYR:CB	1:A:668:LEU:HD13	2.51	0.41
1:A:439:HIS:HE1	3:A:846:HOH:O	2.03	0.40
1:B:599:LYS:HG2	1:B:633:ILE:CG2	2.51	0.40
1:B:643:GLU:HG2	1:B:647:ILE:HD12	2.03	0.40

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	253/275 (92%)	247 (98%)	6 (2%)	0	100	100
1	B	252/275 (92%)	248 (98%)	4 (2%)	0	100	100
All	All	505/550 (92%)	495 (98%)	10 (2%)	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	220/237 (93%)	220 (100%)	0	100	100
1	B	219/237 (92%)	219 (100%)	0	100	100
All	All	439/474 (93%)	439 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	HIS
1	A	506	GLN
1	B	434	GLN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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	255/275 (92%)	0.46	18 (7%)	16	17	20, 32, 56, 73	2 (0%)
1	B	254/275 (92%)	0.53	17 (6%)	17	20	19, 32, 52, 68	0
All	All	509/550 (92%)	0.49	35 (6%)	16	19	19, 32, 53, 73	2 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	556	GLU	4.7
1	B	614	ASP	4.0
1	B	677	ARG	3.9
1	B	430	ARG	3.9
1	A	678	LEU	3.7
1	B	509	ASP	3.6
1	B	610	GLN	3.5
1	B	613	ASP	3.3
1	A	425	LEU	3.2
1	A	613	ASP	3.2
1	B	607	ASP	3.2
1	A	431	ASP	3.0
1	B	427	LYS	2.9
1	A	555	MET	2.9
1	B	424	GLU	2.8
1	A	481	GLN	2.8
1	B	434	GLN	2.7
1	B	556	GLU	2.7
1	A	558	ILE	2.6
1	A	607	ASP	2.6
1	B	426	GLU	2.6
1	B	481	GLN	2.5
1	A	611	ASP	2.4
1	A	430	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	429	LEU	2.4
1	B	558	ILE	2.3
1	A	466	LEU	2.3
1	A	657	TYR	2.3
1	A	467	HIS	2.3
1	B	473	ASP	2.2
1	A	435	ARG	2.1
1	A	428	ASP	2.1
1	A	473	ASP	2.0
1	B	612	GLU	2.0
1	B	555	MET	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	701	1/1	0.75	0.11	27,27,27,27	0
2	MG	A	701	1/1	0.92	0.10	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.