



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6IZS / pdb_00006izs
Title : Crystal structure of Haemophilus influenzae BamA POTRA4
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Deposited on : 2018-12-20
Resolution : 2.03 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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

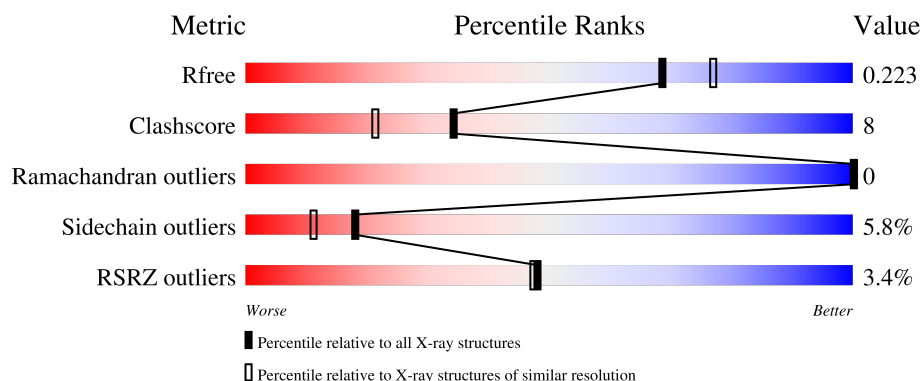
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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 $\leq 5\%$. 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	122	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 753 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	87	Total	C	N	O	S	0	0	0
			656	406	119	129	2			

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P46024
A	2	GLY	-	expression tag	UNP P46024
A	3	SER	-	expression tag	UNP P46024
A	4	SER	-	expression tag	UNP P46024
A	5	HIS	-	expression tag	UNP P46024
A	6	HIS	-	expression tag	UNP P46024
A	7	HIS	-	expression tag	UNP P46024
A	8	HIS	-	expression tag	UNP P46024
A	9	HIS	-	expression tag	UNP P46024
A	10	HIS	-	expression tag	UNP P46024
A	11	SER	-	expression tag	UNP P46024
A	12	SER	-	expression tag	UNP P46024
A	13	GLY	-	expression tag	UNP P46024
A	14	LEU	-	expression tag	UNP P46024
A	15	VAL	-	expression tag	UNP P46024
A	16	PRO	-	expression tag	UNP P46024
A	17	ARG	-	expression tag	UNP P46024
A	18	GLY	-	expression tag	UNP P46024
A	19	SER	-	expression tag	UNP P46024
A	20	HIS	-	expression tag	UNP P46024
A	21	MET	-	expression tag	UNP P46024
A	107	GLY	-	expression tag	UNP P46024
A	108	SER	-	expression tag	UNP P46024
A	109	GLY	-	expression tag	UNP P46024
A	110	SER	-	expression tag	UNP P46024
A	111	GLY	-	expression tag	UNP P46024
A	112	SER	-	expression tag	UNP P46024

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Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLY	-	expression tag	UNP P46024
A	114	VAL	-	expression tag	UNP P46024
A	115	ALA	-	expression tag	UNP P46024
A	116	ALA	-	expression tag	UNP P46024
A	117	GLY	-	expression tag	UNP P46024
A	118	VAL	-	expression tag	UNP P46024
A	119	GLY	-	expression tag	UNP P46024
A	120	TYR	-	expression tag	UNP P46024
A	121	GLN	-	expression tag	UNP P46024
A	122	TRP	-	expression tag	UNP P46024

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	97	Total O 97 97	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	80.53Å 80.53Å 105.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.00 – 2.03 42.00 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.00-2.03) 99.6 (42.00-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.178 , 0.218 0.193 , 0.223	Depositor DCC
R_{free} test set	640 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	753	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	2.04	17/662 (2.6%)	1.64	8/893 (0.9%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	ARG	CA-C	-7.62	1.43	1.52
1	A	84	VAL	CA-CB	7.37	1.60	1.54
1	A	106	LEU	CA-C	6.43	1.61	1.52
1	A	22	LEU	N-CA	6.36	1.54	1.46
1	A	57	ARG	CG-CD	6.03	1.70	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	57	ARG	CB-CG-CD	8.46	130.76	111.30
1	A	47	SER	CA-CB-OG	-7.62	95.86	111.10
1	A	27	ARG	N-CA-C	6.62	120.57	112.23
1	A	57	ARG	CG-CD-NE	6.27	125.80	112.00
1	A	30	ARG	NE-CZ-NH1	-5.30	116.20	121.50

There are no chirality outliers.

There are no planarity outliers.

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	A	656	0	662	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	97	0	0	6	0
All	All	753	0	662	10	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 8.

The worst 5 of 10 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:21:MET:HA	2:A:256:HOH:O	1.81	0.80
1:A:21:MET:N	2:A:201:HOH:O	2.26	0.68
1:A:83:SER:OG	1:A:98:LEU:CD2	2.58	0.51
1:A:50:HIS:HD2	2:A:203:HOH:O	1.94	0.51
1:A:57:ARG:CD	1:A:57:ARG:H	2.27	0.48

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	85/122 (70%)	83 (98%)	2 (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	69/94 (73%)	65 (94%)	4 (6%)	18	11

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

Mol	Chain	Res	Type
1	A	21	MET
1	A	57	ARG
1	A	85	PRO
1	A	105	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS

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 oligosaccharides 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, 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	87/122 (71%)	0.40	3 (3%) 48 47	34, 50, 78, 119	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	GLY	6.0
1	A	21	MET	4.6
1	A	106	LEU	4.6

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 oligosaccharides 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.