



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:40 PM EDT

PDB ID : 3UE3 / pdb_00003ue3
Title : Crystal structure of Acinetobacter baumannii PBP3
Authors : Han, S.
Deposited on : 2011-10-28
Resolution : 2.30 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	:	4-5-2 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

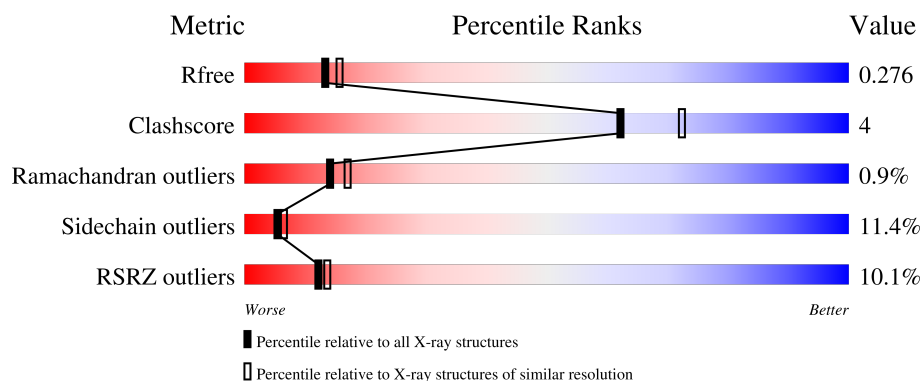
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	554	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3470 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 Septum formation, penicillin binding protein 3, peptidoglycan synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3305	2081	580	628	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	MET	-	expression tag	UNP C0VN42
A	57	SER	-	expression tag	UNP C0VN42
A	58	HIS	-	expression tag	UNP C0VN42
A	59	HIS	-	expression tag	UNP C0VN42
A	60	HIS	-	expression tag	UNP C0VN42
A	61	HIS	-	expression tag	UNP C0VN42
A	62	HIS	-	expression tag	UNP C0VN42
A	63	HIS	-	expression tag	UNP C0VN42

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	165	Total	O	0	0
			165	165		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	39.66Å 89.71Å 211.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.32 – 2.30 38.32 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.32-2.30) 97.8 (38.32-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, R_{free}	0.217 , 0.250 0.236 , 0.276	Depositor DCC
R_{free} test set	1721 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.949	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3470	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 5.95% 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 ⓘ

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	0.87	1/3363 (0.0%)	1.44	32/4552 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	491	ASP	CA-C	5.80	1.59	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	MET	N-CA-C	13.73	126.33	111.36
1	A	323	MET	CA-C-N	11.56	142.50	121.70
1	A	323	MET	C-N-CA	11.56	142.50	121.70
1	A	322	ALA	N-CA-C	7.34	121.48	112.23
1	A	437	LYS	CA-C-N	7.16	135.21	121.54
1	A	437	LYS	C-N-CA	7.16	135.21	121.54
1	A	81	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	450	TYR	N-CA-C	6.87	122.20	113.55
1	A	247	VAL	CA-C-N	6.74	133.84	121.70
1	A	247	VAL	C-N-CA	6.74	133.84	121.70
1	A	263	SER	CA-C-N	6.11	128.69	120.50
1	A	263	SER	C-N-CA	6.11	128.69	120.50
1	A	330	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	371	THR	CB-CA-C	5.83	120.39	109.71
1	A	384	THR	CB-CA-C	5.56	120.02	110.79
1	A	570	GLY	CA-C-N	5.48	127.62	120.28
1	A	570	GLY	C-N-CA	5.48	127.62	120.28
1	A	250	VAL	N-CA-C	5.44	116.61	109.21
1	A	438	LEU	CA-C-N	5.42	131.90	121.54
1	A	438	LEU	C-N-CA	5.42	131.90	121.54
1	A	323	MET	CA-C-O	-5.40	114.70	120.42
1	A	251	ILE	N-CA-C	-5.38	106.45	111.45
1	A	554	VAL	N-CA-C	5.32	117.69	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ALA	N-CA-C	5.30	117.74	111.33
1	A	353	THR	CB-CA-C	5.28	117.24	109.22
1	A	199	PRO	N-CA-C	5.26	123.30	112.47
1	A	438	LEU	N-CA-C	5.25	121.97	110.80
1	A	552	ALA	N-CA-C	5.10	114.69	108.11
1	A	319	ASN	CA-C-N	5.05	131.18	121.54
1	A	319	ASN	C-N-CA	5.05	131.18	121.54
1	A	557	PRO	N-CA-C	5.04	118.79	111.03
1	A	211	SER	N-CA-C	-5.02	105.99	111.82

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	3305	0	3353	27	0
2	A	165	0	0	1	0
All	All	3470	0	3353	27	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 (27) 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:202:ASN:HB3	1:A:206:ILE:HD12	1.83	0.59
1:A:517:ILE:HD12	1:A:522:VAL:HG21	1.83	0.59
1:A:324:ARG:HE	1:A:329:ILE:HD11	1.68	0.58
1:A:436:ASP:C	1:A:438:LEU:H	2.13	0.57
1:A:384:THR:HB	1:A:501:MET:HG2	1.87	0.56
1:A:408:PRO:HD3	1:A:443:LEU:HD11	1.88	0.55
1:A:344:ALA:HB1	1:A:490:LEU:HD11	1.88	0.55
1:A:431:LEU:HB2	1:A:453:ASN:HB2	1.91	0.53
1:A:334:PRO:CG	1:A:338:MET:HG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:HG2	1:A:251:ILE:HD11	1.92	0.50
1:A:367:LEU:HB3	1:A:441:SER:HB2	1.94	0.50
1:A:456:ILE:HG23	1:A:562:ILE:HB	1.95	0.47
1:A:388:VAL:HA	1:A:505:VAL:HG22	1.96	0.47
1:A:223:LEU:HD13	1:A:260:ILE:HD13	1.96	0.47
1:A:526:THR:HG22	1:A:548:PHE:HD2	1.78	0.46
1:A:72:LEU:HD11	1:A:234:GLN:HB2	1.98	0.45
1:A:506:THR:HG21	1:A:522:VAL:HG12	1.98	0.45
1:A:422:VAL:HG23	1:A:475:LEU:HB3	1.99	0.45
1:A:267:ARG:HB3	1:A:592:LEU:HD21	1.99	0.45
1:A:338:MET:HE1	1:A:416:PHE:CZ	2.52	0.45
1:A:451:GLY:HA3	2:A:722:HOH:O	2.17	0.44
1:A:95:LYS:HB3	1:A:189:GLU:HB2	1.99	0.43
1:A:202:ASN:OD1	1:A:269:GLN:HG2	2.19	0.42
1:A:530:HIS:HE1	1:A:573:TYR:OH	2.01	0.42
1:A:334:PRO:HG2	1:A:338:MET:HG2	2.02	0.41
1:A:505:VAL:HG12	1:A:512:ALA:HB3	2.02	0.40
1:A:387:ILE:HD12	1:A:501:MET:SD	2.62	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	430/554 (78%)	413 (96%)	13 (3%)	4 (1%)	14 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	ARG
1	A	320	LYS
1	A	438	LEU

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Mol	Chain	Res	Type
1	A	199	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	352/461 (76%)	312 (89%)	40 (11%)	5 6

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ARG
1	A	73	GLU
1	A	81	ASP
1	A	89	ILE
1	A	93	ILE
1	A	94	MET
1	A	191	SER
1	A	194	ARG
1	A	200	GLN
1	A	205	ILE
1	A	208	LEU
1	A	217	GLU
1	A	233	GLU
1	A	254	VAL
1	A	261	THR
1	A	268	LEU
1	A	276	LEU
1	A	321	ASP
1	A	324	ARG
1	A	329	ILE
1	A	338	MET
1	A	353	THR
1	A	358	VAL
1	A	371	THR
1	A	372	ILE

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Mol	Chain	Res	Type
1	A	384	THR
1	A	404	LYS
1	A	418	GLN
1	A	438	LEU
1	A	443	LEU
1	A	459	LEU
1	A	466	LEU
1	A	475	LEU
1	A	481	ASP
1	A	489	VAL
1	A	499	LEU
1	A	514	GLN
1	A	551	VAL
1	A	577	VAL
1	A	602	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	210	ASN
1	A	222	GLN
1	A	234	GLN
1	A	418	GLN
1	A	497	GLN
1	A	504	GLN
1	A	514	GLN
1	A	530	HIS
1	A	587	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 [i](#)

There are no oligosaccharides 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	436/554 (78%)	0.54	44 (10%) 12 14	14, 28, 74, 91	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	438	LEU	7.2
1	A	317	LEU	6.8
1	A	247	VAL	6.6
1	A	250	VAL	5.5
1	A	320	LYS	5.4
1	A	233	GLU	5.3
1	A	186	VAL	5.1
1	A	532	LEU	4.9
1	A	314	LYS	4.6
1	A	246	LYS	4.6
1	A	319	ASN	4.5
1	A	69	THR	4.3
1	A	316	GLY	4.3
1	A	96	ILE	4.1
1	A	321	ASP	4.1
1	A	602	ASP	3.9
1	A	318	SER	3.8
1	A	322	ALA	3.6
1	A	236	ILE	3.6
1	A	248	SER	3.5
1	A	481	ASP	3.3
1	A	249	GLU	3.2
1	A	235	LYS	3.1
1	A	187	TYR	3.0
1	A	315	GLY	3.0
1	A	95	LYS	2.8
1	A	436	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	369	TRP	2.8
1	A	216	ILE	2.8
1	A	323	MET	2.8
1	A	424	PHE	2.6
1	A	313	ASP	2.5
1	A	254	VAL	2.5
1	A	324	ARG	2.5
1	A	536	ARG	2.5
1	A	91	THR	2.4
1	A	252	LYS	2.3
1	A	539	TYR	2.3
1	A	456	ILE	2.3
1	A	213	GLY	2.2
1	A	253	GLU	2.2
1	A	208	LEU	2.1
1	A	251	ILE	2.0
1	A	93	ILE	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 oligosaccharides 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.