



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:22 AM UTC

PDB ID : 6KMO / pdb_00006kmo
Title : Crystal structure of a novel esterase CinB from Enterobacter asburiae
Authors : Shang, F.; Xu, Y.
Deposited on : 2019-07-31
Resolution : 1.45 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

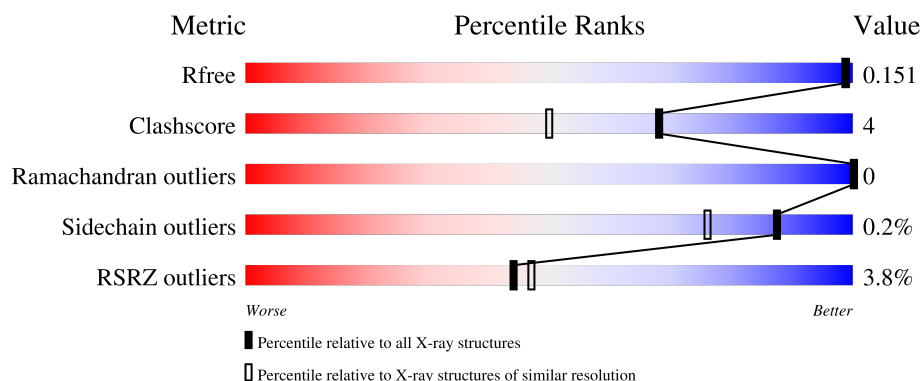
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	337	4% 91% 7%
1	B	337	4% 92% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11098 atoms, of which 5075 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 Alpha/beta hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	330	Total	C	H	N	O	S	0	17	0
			5148	1640	2568	446	486	8			
1	B	328	Total	C	H	N	O	S	0	9	0
			5039	1607	2507	438	479	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ILE	VAL	engineered mutation	UNP A0A1D3AXI2
A	23	ALA	THR	engineered mutation	UNP A0A1D3AXI2
B	9	ILE	VAL	engineered mutation	UNP A0A1D3AXI2
B	23	ALA	THR	engineered mutation	UNP A0A1D3AXI2

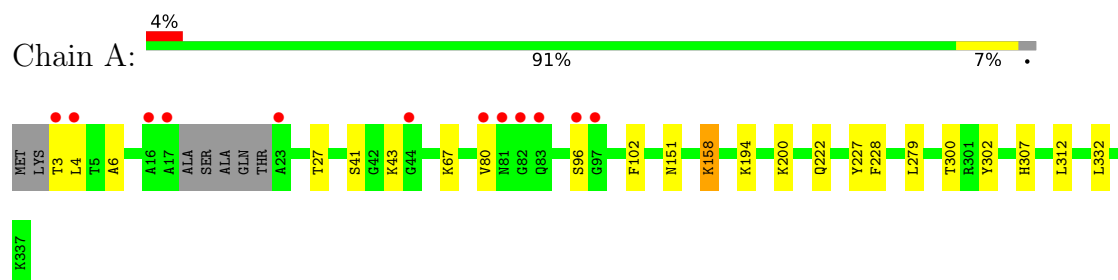
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	460	Total	O	0	0
			460	460		
2	B	451	Total	O	0	0
			451	451		

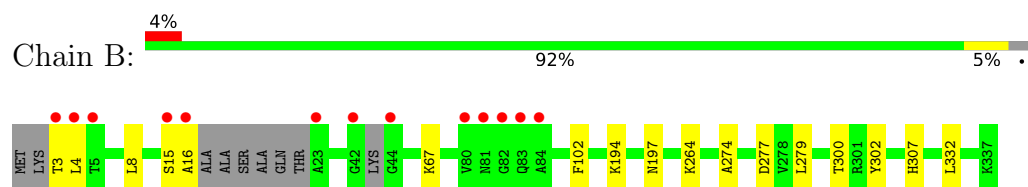
3 Residue-property plots [i](#)

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: Alpha/beta hydrolase



- Molecule 1: Alpha/beta hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.09Å 89.40Å 68.93Å 90.00° 111.26° 90.00°	Depositor
Resolution (Å)	36.69 – 1.45 36.69 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.2 (36.69-1.45) 99.2 (36.69-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.127 , 0.151 0.128 , 0.151	Depositor DCC
R_{free} test set	1994 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å ²)	8.8	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.6	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	0.97	EDS
Total number of atoms	11098	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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	0.36	0/2712	0.57	0/3690
1	B	0.36	0/2622	0.56	0/3567
All	All	0.36	0/5334	0.56	0/7257

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 [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	2580	2568	2488	23	0
1	B	2532	2507	2464	17	2
2	A	460	0	0	6	3
2	B	451	0	0	6	3
All	All	6023	5075	4952	37	5

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 (37) 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:67:LYS:NZ	2:B:401:HOH:O	1.94	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASN:OD1	1:B:4:LEU:HD13	1.80	0.82
1:A:4:LEU:HD21	2:B:455:HOH:O	1.96	0.66
1:A:96:SER:OG	2:A:501:HOH:O	1.80	0.64
1:A:4:LEU:HD11	2:B:435:HOH:O	1.98	0.63
1:A:4:LEU:CD2	2:B:455:HOH:O	2.49	0.58
1:A:158[A]:LYS:NZ	2:A:508:HOH:O	2.39	0.56
1:B:15:SER:OG	1:B:16:ALA:N	2.40	0.55
1:A:302:TYR:CE2	1:B:300[C]:THR:HG22	2.42	0.54
1:B:4:LEU:HD23	1:B:4:LEU:O	2.07	0.54
1:A:300[B]:THR:HG22	1:B:302:TYR:CE2	2.44	0.52
1:B:102:PHE:CD2	1:B:332:LEU:HD21	2.45	0.51
1:A:41:SER:O	1:A:43:LYS:HE2	2.12	0.50
1:B:4:LEU:CD2	1:B:8:LEU:HG	2.42	0.50
1:A:222:GLN:OE1	2:A:502:HOH:O	2.20	0.49
1:A:67:LYS:O	2:A:503:HOH:O	2.20	0.47
1:A:4:LEU:HD13	2:B:436:HOH:O	2.14	0.47
1:B:4:LEU:HD22	1:B:8:LEU:HD11	1.96	0.46
1:A:227:TYR:O	1:A:228[B]:PHE:HB3	2.15	0.46
1:A:194[A]:LYS:NZ	2:A:514:HOH:O	2.49	0.46
1:B:4:LEU:HD22	1:B:8:LEU:CD1	2.47	0.44
1:B:194[A]:LYS:NZ	2:B:413:HOH:O	2.50	0.44
1:A:3:THR:N	1:A:6:ALA:H	2.16	0.44
1:A:102:PHE:CD2	1:A:332[A]:LEU:HD21	2.53	0.44
1:A:228[B]:PHE:CE2	1:A:312:LEU:HD11	2.52	0.43
1:A:4:LEU:O	1:A:4:LEU:HD23	2.19	0.43
1:B:4:LEU:HD22	1:B:8:LEU:HG	2.01	0.43
1:B:279:LEU:HD12	1:B:307:HIS:CE1	2.53	0.43
1:B:4:LEU:HD22	1:B:8:LEU:CG	2.50	0.42
1:A:27[A]:THR:HG21	2:A:830:HOH:O	2.19	0.42
1:A:80:VAL:HG23	1:A:80:VAL:O	2.19	0.42
1:B:194[B]:LYS:HE2	1:B:264:LYS:O	2.19	0.42
1:A:200:LYS:HD3	1:A:200:LYS:HA	1.71	0.42
1:A:279:LEU:HD12	1:A:307:HIS:CE1	2.55	0.42
1:A:43:LYS:HA	1:A:43:LYS:HD3	1.87	0.41
1:B:274:ALA:HB3	1:B:277:ASP:HB2	2.02	0.41
1:B:4:LEU:HD23	1:B:4:LEU:C	2.45	0.41

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:THR:OG1	1:B:197:ASN:HD22[1_454]	1.29	0.31
2:A:858:HOH:O	2:B:611:HOH:O[2_745]	2.06	0.14
1:B:3:THR:OG1	1:B:197:ASN:ND2[1_454]	2.10	0.10
2:A:524:HOH:O	2:B:427:HOH:O[2_746]	2.17	0.03
2:A:820:HOH:O	2:B:727:HOH:O[1_455]	2.17	0.03

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	343/337 (102%)	333 (97%)	10 (3%)	0	100	100
1	B	331/337 (98%)	325 (98%)	6 (2%)	0	100	100
All	All	674/674 (100%)	658 (98%)	16 (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	277/266 (104%)	275 (99%)	2 (1%)	76	54
1	B	269/266 (101%)	269 (100%)	0	100	100
All	All	546/532 (103%)	544 (100%)	2 (0%)	87	70

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158[A]	LYS
1	A	158[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	83	GLN
1	A	145	HIS
1	A	225	ASN
1	B	33	GLN
1	B	57	GLN
1	B	81	ASN
1	B	83	GLN
1	B	333	HIS

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 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 ⓘ

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	330/337 (97%)	-0.64	12 (3%)	46 48	3, 10, 31, 53	9 (2%)
1	B	328/337 (97%)	-0.57	13 (3%)	42 45	3, 11, 32, 57	5 (1%)
All	All	658/674 (97%)	-0.60	25 (3%)	44 47	3, 10, 32, 57	14 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	LEU	7.3
1	A	4	LEU	6.3
1	B	16	ALA	5.4
1	B	44	GLY	5.4
1	A	3	THR	5.1
1	A	17	ALA	5.1
1	B	23	ALA	4.7
1	B	3	THR	4.4
1	A	96	SER	3.7
1	A	23	ALA	3.3
1	B	80	VAL	3.2
1	A	16[A]	ALA	3.1
1	B	83	GLN	3.0
1	B	84	ALA	2.9
1	A	80	VAL	2.9
1	B	5	THR	2.8
1	B	42	GLY	2.7
1	B	81	ASN	2.6
1	A	83	GLN	2.5
1	A	97	GLY	2.5
1	B	82	GLY	2.5
1	A	81	ASN	2.4
1	A	82	GLY	2.3
1	A	44	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	15	SER	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.