



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:21 AM UTC

PDB ID : 5Z16 / pdb_00005z16
Title : A novel dimeric isocitrate dehydrogenase from *Acinetobacter baumannii*
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Deposited on : 2017-12-25
Resolution : 3.00 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
Mogul : 2022.3.0, CSD as543be (2022)
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

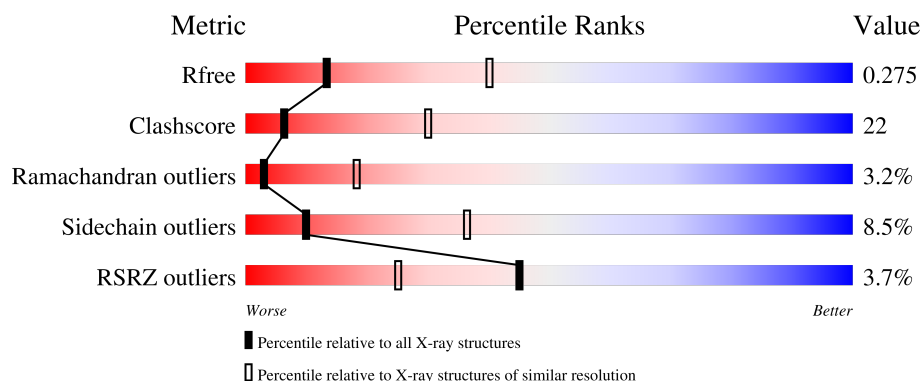
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	751	
1	B	751	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11788 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 Isocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	0
			5666	3571	969	1091	35			
1	B	739	Total	C	N	O	S	0	0	0
			5741	3626	978	1102	35			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP V5VCI0
A	-4	HIS	-	expression tag	UNP V5VCI0
A	-3	HIS	-	expression tag	UNP V5VCI0
A	-2	HIS	-	expression tag	UNP V5VCI0
A	-1	HIS	-	expression tag	UNP V5VCI0
A	0	HIS	-	expression tag	UNP V5VCI0
A	629	THR	ALA	conflict	UNP V5VCI0
B	-5	HIS	-	expression tag	UNP V5VCI0
B	-4	HIS	-	expression tag	UNP V5VCI0
B	-3	HIS	-	expression tag	UNP V5VCI0
B	-2	HIS	-	expression tag	UNP V5VCI0
B	-1	HIS	-	expression tag	UNP V5VCI0
B	0	HIS	-	expression tag	UNP V5VCI0
B	629	THR	ALA	conflict	UNP V5VCI0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

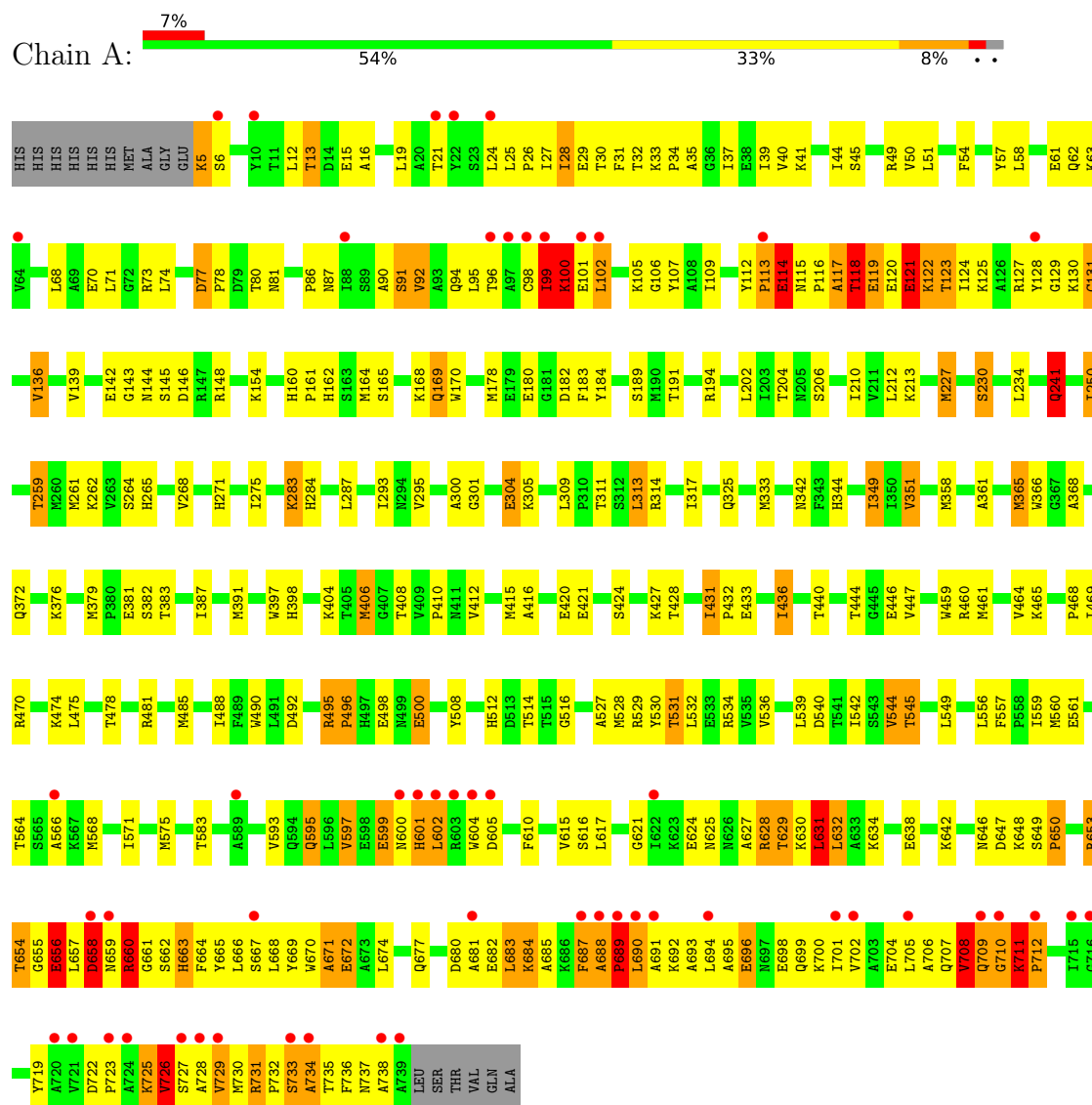
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	201	Total	O	0	0
			201	201		
4	B	168	Total	O	0	0
			168	168		

3 Residue-property plots

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: Isocitrate dehydrogenase



• Molecule 1: Isocitrate dehydrogenase



I715	L602	L491	Y373	K257	D111	HIS
Y718	R603	L491	Y373	A258	D111	HIS
V721	E609	D492	M379	T259	A117	HIS
V726	L613	P493	P380	M260	T118	HIS
V729	V615	H497	E381	M261	E119	HIS
R730	E619	E498	S382	I267	E120	HIS
R731	M620	N499	S382	I267	E121	MET
T742	K623	E500	I387	I275	K122	ALA
V743	G626	L509	Y388	Y276	K122	ALA
Q744	N626	L509	Q389	Y277	T123	GLY
ALA	T629	T515	E390	Y277	I124	GLU
	K634	G516	K396	F281	R127	LYS
	T629	L517	N400	E282	N137	S6
	K634	L517	F401	K283	P138	T11
	T635	I521	D402	H284		L12
	L636	M522	P403	G285		T13
	D637	S523	K404	K286		D14
	T640	Q524		N294	G143	A16
	L643	V525		V295	N144	L19
	K648	R526	T408	N296	S145	A20
	R652	A527	V409		R148	T21
	R653	M528	P410	M299	Y22	Y22
	T654	T531	L414	A300	P150	S23
	L657	R534	M415	G301		L24
	D658	V535	A416	L302	V153	L24
	N659	V536		Y303		L25
	R660	I547	P432	E304	S171	P26
	G661	I548		K305		I27
	S662	L549		I306	H174	I28
	H663	R550	I436		V175	K33
	F664	D551	A437	T311		P34
	Y665	D551			F183	
	L668	D555	L442	R314		I37
	L674	E561			S189	
	F687	S570	T450	I317	M190	I44
	A693	M575	Q451	I318	T191	I44
	N697	E582	R452	E319		V46
	L705	S588	V453	R328	M200	
	A706	V593	E454		T204	V50
	Q707	L596	E455	S336	N205	E53
	V708	V597	R460	N342	S206	
	K711	H601	M461			S59
			C462			
					I223	
					I224	
					D225	Q62
					S226	Q76
					M227	
					Y238	I83
					D244	S91
					I250	Q94
					L254	K100
					H255	
					V256	G106

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.16Å 137.16Å 238.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 3.00 48.54 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.54-3.00) 99.9 (48.54-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.205 , 0.276 0.210 , 0.275	Depositor DCC
R_{free} test set	2267 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11788	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.70	2/5773 (0.0%)	1.19	50/7810 (0.6%)
1	B	0.63	0/5855	0.99	12/7923 (0.2%)
All	All	0.66	2/11628 (0.0%)	1.09	62/15733 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	HIS	CE1-NE2	-8.96	1.23	1.32
1	A	160	HIS	CD2-NE2	8.64	1.47	1.37

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	711	LYS	CA-C-N	-15.35	100.65	119.84
1	A	711	LYS	C-N-CA	-15.35	100.65	119.84
1	A	119	GLU	N-CA-C	9.92	128.86	113.28
1	A	689	PRO	N-CA-C	-9.41	93.08	112.47
1	A	709	GLN	N-CA-C	9.36	130.74	110.80

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	5666	0	5620	380	0
1	B	5741	0	5699	126	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	201	0	0	22	0
4	B	168	0	0	22	0
All	All	11788	0	11319	503	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 22.

The worst 5 of 503 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:24:LEU:CD2	1:A:663:HIS:ND1	1.81	1.43
1:A:24:LEU:HD23	1:A:663:HIS:ND1	1.14	1.40
1:A:688:ALA:C	1:A:690:LEU:H	1.04	1.39
1:A:96:THR:HA	1:A:99:ILE:CG2	1.56	1.35
1:A:96:THR:O	1:A:100:LYS:HD2	1.25	1.31

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	733/751 (98%)	626 (85%)	70 (10%)	37 (5%)	1	10
1	B	737/751 (98%)	673 (91%)	54 (7%)	10 (1%)	9	36
All	All	1470/1502 (98%)	1299 (88%)	124 (8%)	47 (3%)	3	18

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	GLU
1	A	117	ALA
1	A	647	ASP
1	A	654	THR
1	A	658	ASP

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	601/628 (96%)	548 (91%)	53 (9%)	9	35
1	B	614/628 (98%)	564 (92%)	50 (8%)	11	38
All	All	1215/1256 (97%)	1112 (92%)	103 (8%)	10	36

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	83	ILE
1	B	259	THR
1	B	652	ARG
1	B	120	GLU
1	B	191	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	646	ASN
1	B	372	GLN
1	A	663	HIS
1	B	512	HIS
1	B	296	ASN

5.3.3 RNA ⓘ

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	B	801	-	4,4,4	1.02	0	6,6,6	0.67	0
2	PO4	A	801	-	4,4,4	0.92	0	6,6,6	0.67	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PO4	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	735/751 (97%)	0.23	53 (7%)	21 11	28, 50, 130, 141	0
1	B	739/751 (98%)	-0.46	1 (0%)	92 86	22, 38, 64, 100	0
All	All	1474/1502 (98%)	-0.11	54 (3%)	45 25	22, 42, 125, 141	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	605	ASP	7.4
1	A	728	ALA	6.8
1	A	101	GLU	5.9
1	A	22	TYR	5.8
1	A	739	ALA	4.9

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](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	PO4	A	801	5/5	0.94	0.08	52,53,59,66	0
3	MG	A	802	1/1	0.95	0.14	27,27,27,27	0
3	MG	B	802	1/1	0.95	0.15	38,38,38,38	0
2	PO4	B	801	5/5	0.96	0.09	41,41,49,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.