



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:50 AM UTC

PDB ID : 3F72 / pdb_00003f72
Title : Crystal Structure of the Staphylococcus aureus pI258 CadC Metal Binding Site 2 Mutant
Authors : Kandegedara, A.; Thiyagarajan, S.; Kondapalli, K.C.; Stemmler, T.L.; Rosen, B.P.
Deposited on : 2008-11-07
Resolution : 2.31 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

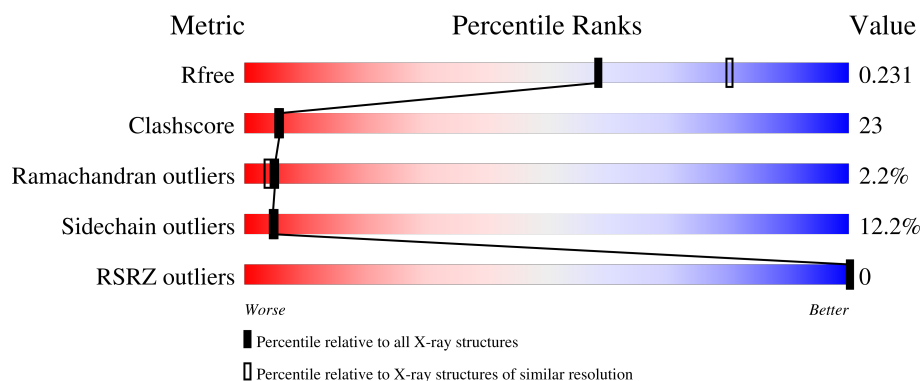
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	122	
1	B	122	
1	C	122	
1	D	122	
1	E	122	

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Mol	Chain	Length	Quality of chain
1	F	122	40% 30% 11% • 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4843 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 Cadmium efflux system accessory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	0	0	0
			821	517	145	154	5			
1	B	108	Total	C	N	O	S	0	0	0
			832	521	147	159	5			
1	C	103	Total	C	N	O	S	0	0	0
			797	500	142	150	5			
1	D	100	Total	C	N	O	S	0	0	0
			761	479	130	147	5			
1	E	101	Total	C	N	O	S	0	0	0
			737	459	126	147	5			
1	F	102	Total	C	N	O	S	0	0	0
			748	465	130	148	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	CYS	engineered mutation	UNP P20047
A	101	GLY	ASP	engineered mutation	UNP P20047
A	103	ALA	HIS	engineered mutation	UNP P20047
B	11	GLY	CYS	engineered mutation	UNP P20047
B	101	GLY	ASP	engineered mutation	UNP P20047
B	103	ALA	HIS	engineered mutation	UNP P20047
C	11	GLY	CYS	engineered mutation	UNP P20047
C	101	GLY	ASP	engineered mutation	UNP P20047
C	103	ALA	HIS	engineered mutation	UNP P20047
D	11	GLY	CYS	engineered mutation	UNP P20047
D	101	GLY	ASP	engineered mutation	UNP P20047
D	103	ALA	HIS	engineered mutation	UNP P20047
E	11	GLY	CYS	engineered mutation	UNP P20047
E	101	GLY	ASP	engineered mutation	UNP P20047
E	103	ALA	HIS	engineered mutation	UNP P20047
F	11	GLY	CYS	engineered mutation	UNP P20047
F	101	GLY	ASP	engineered mutation	UNP P20047

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Chain	Residue	Modelled	Actual	Comment	Reference
F	103	ALA	HIS	engineered mutation	UNP P20047

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is water.

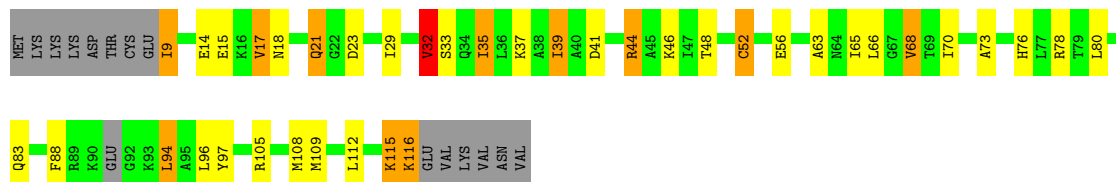
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	26	Total O 26 26	0	0
3	B	27	Total O 27 27	0	0
3	C	25	Total O 25 25	0	0
3	D	24	Total O 24 24	0	0
3	E	24	Total O 24 24	0	0
3	F	16	Total O 16 16	0	0

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.

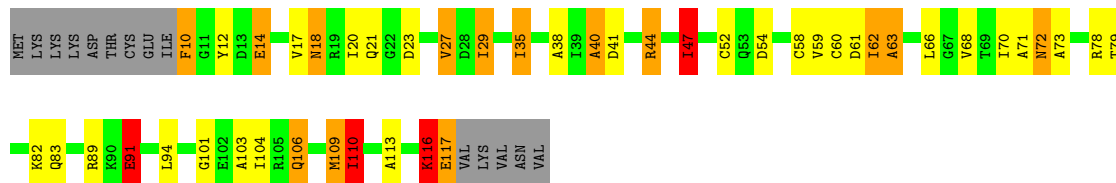
• Molecule 1: Cadmium efflux system accessory protein

Chain A: 

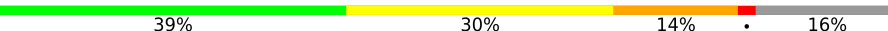


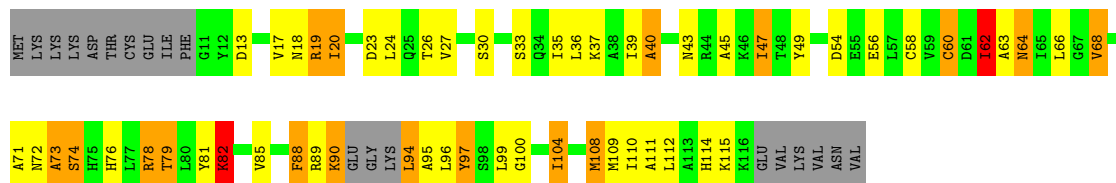
• Molecule 1: Cadmium efflux system accessory protein

Chain B: 

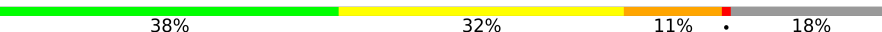


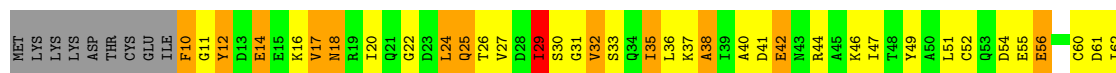
• Molecule 1: Cadmium efflux system accessory protein

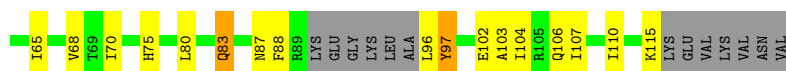
Chain C: 



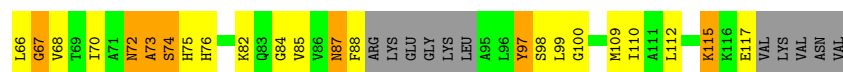
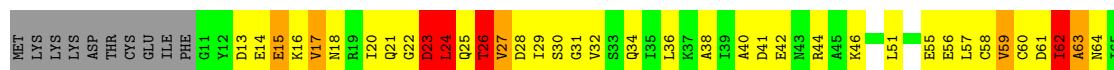
• Molecule 1: Cadmium efflux system accessory protein

Chain D: 

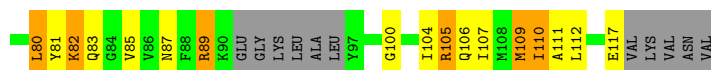




- Molecule 1: Cadmium efflux system accessory protein



- Molecule 1: Cadmium efflux system accessory protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	89.47Å 89.47Å 148.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.30 – 2.31 34.30 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.3 (34.30-2.31) 97.4 (34.30-2.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.237 , 0.288 (Not available) , 0.231	Depositor DCC
R_{free} test set	2539 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.366 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4843	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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](#)

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

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	1.83	12/828 (1.4%)	1.64	11/1114 (1.0%)
1	B	2.01	16/840 (1.9%)	1.77	17/1130 (1.5%)
1	C	1.93	14/803 (1.7%)	1.83	19/1079 (1.8%)
1	D	1.72	10/768 (1.3%)	1.60	10/1037 (1.0%)
1	E	1.74	11/742 (1.5%)	1.62	8/1006 (0.8%)
1	F	1.62	7/754 (0.9%)	1.65	12/1021 (1.2%)
All	All	1.82	70/4735 (1.5%)	1.69	77/6387 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	2
All	All	0	3

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	17	VAL	CA-CB	9.10	1.65	1.54
1	A	70	ILE	CA-CB	8.31	1.64	1.54
1	B	63	ALA	CA-CB	8.20	1.66	1.53
1	A	17	VAL	C-O	7.87	1.32	1.24
1	E	26	THR	CA-C	7.83	1.63	1.52

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ILE	N-CA-C	-9.76	101.05	110.42
1	C	82	LYS	N-CA-C	-9.58	99.91	111.69
1	C	95	ALA	N-CA-C	9.01	122.92	108.41
1	C	40	ALA	N-CA-C	8.63	121.47	111.11
1	C	62	ILE	N-CA-C	8.37	119.16	110.62

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	91	GLU	Peptide
1	E	26	THR	Peptide
1	E	87	ASN	Peptide

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	821	0	834	31	0
1	B	832	0	838	37	0
1	C	797	0	820	50	0
1	D	761	0	754	45	0
1	E	737	0	701	54	0
1	F	748	0	707	35	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	F	1	0	0	0	0
3	A	26	0	0	6	0
3	B	27	0	0	0	0
3	C	25	0	0	1	0
3	D	24	0	0	3	0
3	E	24	0	0	1	0
3	F	16	0	0	3	0
All	All	4843	0	4654	215	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 23.

The worst 5 of 215 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:E:24:LEU:N	1:E:25:GLN:HA	1.36	1.23
1:E:23:ASP:HB3	1:E:25:GLN:CA	1.70	1.20
1:B:47:ILE:HD11	1:B:66:LEU:HD11	1.25	1.18
1:E:20:ILE:HD11	1:F:54:ASP:OD1	1.51	1.11
1:E:23:ASP:HB3	1:E:25:GLN:CB	1.80	1.10

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	103/122 (84%)	96 (93%)	7 (7%)	0	100	100
1	B	106/122 (87%)	100 (94%)	6 (6%)	0	100	100
1	C	99/122 (81%)	91 (92%)	7 (7%)	1 (1%)	12	14
1	D	96/122 (79%)	88 (92%)	7 (7%)	1 (1%)	12	14
1	E	97/122 (80%)	83 (86%)	7 (7%)	7 (7%)	1	0
1	F	98/122 (80%)	85 (87%)	9 (9%)	4 (4%)	2	1
All	All	599/732 (82%)	543 (91%)	43 (7%)	13 (2%)	5	4

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	23	ASP
1	E	24	LEU
1	E	73	ALA
1	E	16	LYS
1	F	65	ILE

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	86/103 (84%)	81 (94%)	5 (6%)	18	25
1	B	87/103 (84%)	77 (88%)	10 (12%)	5	6
1	C	85/103 (82%)	75 (88%)	10 (12%)	5	5
1	D	80/103 (78%)	72 (90%)	8 (10%)	7	8
1	E	73/103 (71%)	60 (82%)	13 (18%)	2	1
1	F	74/103 (72%)	61 (82%)	13 (18%)	2	2
All	All	485/618 (78%)	426 (88%)	59 (12%)	5	5

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	27	VAL
1	F	87	ASN
1	E	23	ASP
1	F	59	VAL
1	F	29	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	72	ASN
1	E	76	HIS
1	F	53	GLN
1	F	18	ASN
1	C	53	GLN

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 5 ligands modelled in this entry, 5 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 [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 [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	107/122 (87%)	-1.10	0 100 100	34, 48, 73, 81	0
1	B	108/122 (88%)	-1.19	0 100 100	26, 42, 68, 78	1 (0%)
1	C	103/122 (84%)	-1.01	0 100 100	36, 53, 71, 75	0
1	D	100/122 (81%)	-1.00	0 100 100	37, 55, 76, 82	0
1	E	101/122 (82%)	-0.95	0 100 100	42, 60, 83, 91	0
1	F	102/122 (83%)	-0.97	0 100 100	42, 66, 86, 91	0
All	All	621/732 (84%)	-1.04	0 100 100	26, 54, 79, 91	1 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	NA	B	123	1/1	0.98	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	F	123	1/1	0.98	0.16	69,69,69,69	0
2	NA	A	123	1/1	0.99	0.05	41,41,41,41	0
2	NA	B	124	1/1	0.99	0.17	55,55,55,55	0
2	NA	A	124	1/1	0.99	0.17	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.