



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:07 AM UTC

PDB ID : 3KHX / pdb_00003khx
Title : Crystal structure of Staphylococcus aureus metallopeptidase (Sapep/DapE) in the apo-form
Authors : Girish, T.S.; Gopal, B.
Deposited on : 2009-10-31
Resolution : 2.30 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

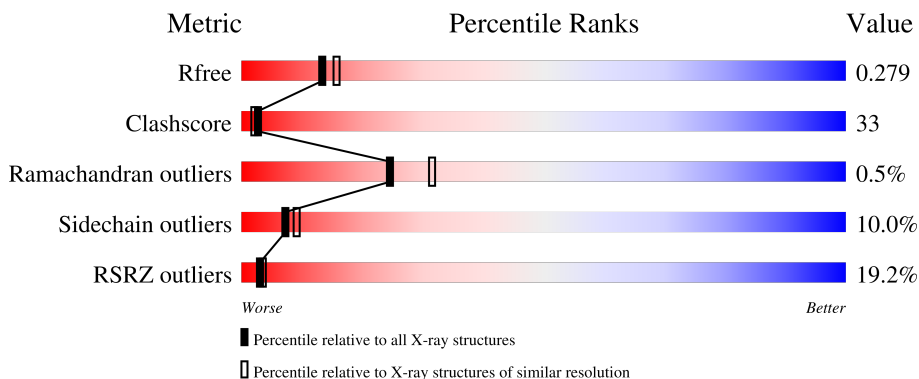
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	492	
1	B	492	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6716 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 Putative dipeptidase SACOL1801.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	422	3232	2052	531	635	14	1	0	0
1	B	425	3302	2099	546	642	15	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q5HF23
A	-21	GLY	-	expression tag	UNP Q5HF23
A	-20	SER	-	expression tag	UNP Q5HF23
A	-19	SER	-	expression tag	UNP Q5HF23
A	-18	HIS	-	expression tag	UNP Q5HF23
A	-17	HIS	-	expression tag	UNP Q5HF23
A	-16	HIS	-	expression tag	UNP Q5HF23
A	-15	HIS	-	expression tag	UNP Q5HF23
A	-14	HIS	-	expression tag	UNP Q5HF23
A	-13	HIS	-	expression tag	UNP Q5HF23
A	-12	SER	-	expression tag	UNP Q5HF23
A	-11	SER	-	expression tag	UNP Q5HF23
A	-10	GLY	-	expression tag	UNP Q5HF23
A	-9	LEU	-	expression tag	UNP Q5HF23
A	-8	VAL	-	expression tag	UNP Q5HF23
A	-7	PRO	-	expression tag	UNP Q5HF23
A	-6	ARG	-	expression tag	UNP Q5HF23
A	-5	GLY	-	expression tag	UNP Q5HF23
A	-4	SER	-	expression tag	UNP Q5HF23
A	-3	HIS	-	expression tag	UNP Q5HF23
A	-2	MET	-	expression tag	UNP Q5HF23
A	-1	ALA	-	expression tag	UNP Q5HF23
A	0	SER	-	expression tag	UNP Q5HF23
B	-22	MET	-	expression tag	UNP Q5HF23
B	-21	GLY	-	expression tag	UNP Q5HF23

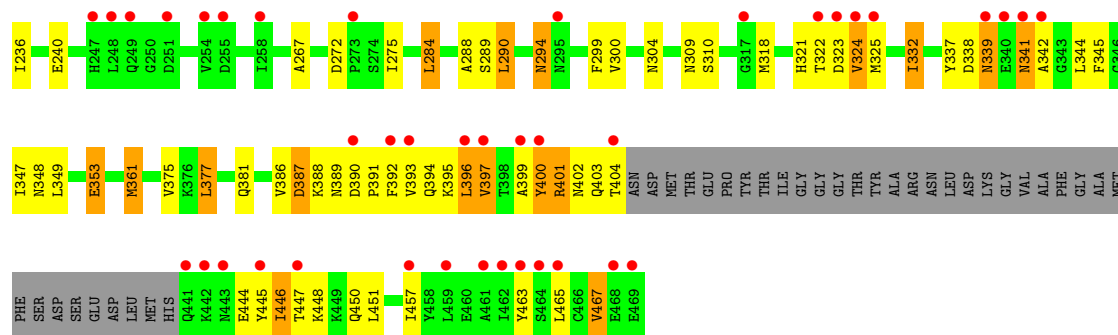
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	expression tag	UNP Q5HF23
B	-19	SER	-	expression tag	UNP Q5HF23
B	-18	HIS	-	expression tag	UNP Q5HF23
B	-17	HIS	-	expression tag	UNP Q5HF23
B	-16	HIS	-	expression tag	UNP Q5HF23
B	-15	HIS	-	expression tag	UNP Q5HF23
B	-14	HIS	-	expression tag	UNP Q5HF23
B	-13	HIS	-	expression tag	UNP Q5HF23
B	-12	SER	-	expression tag	UNP Q5HF23
B	-11	SER	-	expression tag	UNP Q5HF23
B	-10	GLY	-	expression tag	UNP Q5HF23
B	-9	LEU	-	expression tag	UNP Q5HF23
B	-8	VAL	-	expression tag	UNP Q5HF23
B	-7	PRO	-	expression tag	UNP Q5HF23
B	-6	ARG	-	expression tag	UNP Q5HF23
B	-5	GLY	-	expression tag	UNP Q5HF23
B	-4	SER	-	expression tag	UNP Q5HF23
B	-3	HIS	-	expression tag	UNP Q5HF23
B	-2	MET	-	expression tag	UNP Q5HF23
B	-1	ALA	-	expression tag	UNP Q5HF23
B	0	SER	-	expression tag	UNP Q5HF23

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	92	Total O 92 92	0	0
2	B	90	Total O 90 90	0	0



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.82Å 134.17Å 68.28Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	60.71 – 2.30 60.71 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (60.71-2.30) 99.3 (60.71-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.246 , 0.278 0.256 , 0.279	Depositor DCC
R_{free} test set	2605 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtrriage
Anisotropy	0.134	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for l,-k,h	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6716	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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	0.72	0/3298	1.00	16/4478 (0.4%)
1	B	0.65	0/3372	0.93	15/4574 (0.3%)
All	All	0.69	0/6670	0.96	31/9052 (0.3%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	VAL	CB-CA-C	-8.22	104.72	111.71
1	A	39	GLY	CA-C-N	7.54	126.81	118.97
1	A	39	GLY	C-N-CA	7.54	126.81	118.97
1	A	211	SER	CB-CA-C	7.43	120.74	110.34
1	B	341	ASN	N-CA-C	7.22	118.84	110.97

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	3232	0	3017	211	0
1	B	3302	0	3113	210	0
2	A	92	0	0	8	0
2	B	90	0	0	4	0
All	All	6716	0	6130	421	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 33.

The worst 5 of 421 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:185:ILE:HB	1:A:350:ARG:NH1	1.28	1.43
1:A:130:LEU:HD21	1:A:459:LEU:CD1	1.55	1.34
1:A:186:THR:CG2	1:A:380:VAL:HG22	1.60	1.32
1:B:5:LYS:N	1:B:5:LYS:HE3	1.50	1.27
1:A:114:LEU:HD11	1:A:445:TYR:O	1.35	1.25

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	414/492 (84%)	397 (96%)	15 (4%)	2 (0%)	24	31
1	B	417/492 (85%)	399 (96%)	16 (4%)	2 (0%)	24	31
All	All	831/984 (84%)	796 (96%)	31 (4%)	4 (0%)	24	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	VAL
1	B	110	ALA
1	A	343	GLY
1	B	324	VAL

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	330/418 (79%)	296 (90%)	34 (10%)	7 8
1	B	343/418 (82%)	310 (90%)	33 (10%)	8 10
All	All	673/836 (80%)	606 (90%)	67 (10%)	7 9

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	332	ILE
1	B	353	GLU
1	B	400	TYR
1	A	341	ASN
1	A	340	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	403	GLN
1	B	453	ASN
1	B	76	ASN
1	B	384	HIS
1	B	12	GLN

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 [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	422/492 (85%)	1.27	89 (21%) 2 3	31, 49, 76, 95	1 (0%)
1	B	425/492 (86%)	1.17	74 (17%) 4 4	29, 47, 83, 110	0
All	All	847/984 (86%)	1.22	163 (19%) 3 3	29, 48, 80, 110	1 (0%)

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	THR	6.9
1	A	405	ASN	5.9
1	B	404	THR	5.5
1	A	267	ALA	5.2
1	A	465	LEU	4.7

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.