



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:00 AM GMT

PDB ID : 3KHZ
Title : Crystal Structure of R350A mutant of Staphylococcus aureus metallopeptidase (Sapep/DapE) in the apo-form
Authors : Girish, T.S.; Gopal, B.
Deposited on : 2009-10-31
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

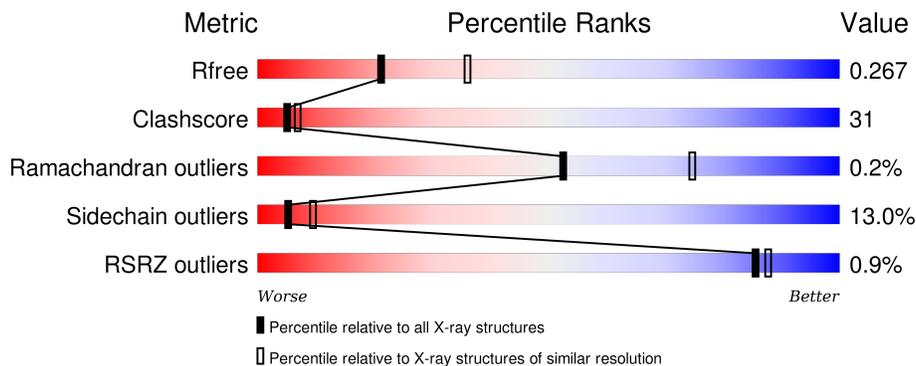
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	 54% 27% 6% 12%
1	B	492	 52% 29% 7% 12%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6880 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	433	3382	2154	558	655	15	17	0	0
1	B	435	3385	2153	552	664	16	2	0	0

There are 48 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
A	350	ALA	ARG	ENGINEERED MUTATION	UNP Q5HF23
B	-22	MET	-	EXPRESSION TAG	UNP Q5HF23

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	GLY	-	EXPRESSION TAG	UNP Q5HF23
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
B	350	ALA	ARG	ENGINEERED MUTATION	UNP Q5HF23

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	69	Total O 69 69	0	0
2	B	44	Total O 44 44	0	0

E367	ASP
L368	LEU
F373	MET
E374	H440
V375	Q441
K376	K442
L377	M443
G378	E444
K379	Y445
Y380	I446
D387	T447
K388	K448
F391	K449
F392	Q450
Y393	N453
Q394	S456
K395	I457
L396	E460
Y397	Y463
T398	S464
A399	L465
Y400	C466
R401	V467
I402	E468
Q403	GLU
T404	GLU
ASN	ASP
ASP	MET
MET	THR
THR	GLU
GLU	PRO
PRO	TYR
TYR	THR
THR	THR
THR	ILE
ILE	GLY
GLY	GLY
GLY	THR
THR	TYR
TYR	ALA
ALA	ARG
ARG	ASN
ASN	LEU
LEU	ASP
ASP	LYS
LYS	GLY
GLY	VAL
VAL	ALA
ALA	PHE
PHE	GLY
GLY	ALA
ALA	MET
MET	PHE
PHE	SER
SER	ASP
ASP	SER
SER	SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.75Å 133.52Å 67.71Å 90.00° 95.59° 90.00°	Depositor
Resolution (Å)	49.02 – 2.50 49.02 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.02-2.50) 100.0 (49.02-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.24 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.208 , 0.269 0.215 , 0.267	Depositor DCC
R_{free} test set	1984 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	EDS
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 39560 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6880	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.68	0/3457	0.72	4/4691 (0.1%)
1	B	0.67	0/3460	0.70	1/4700 (0.0%)
All	All	0.67	0/6917	0.71	5/9391 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	LEU	CA-CB-CG	5.84	128.73	115.30
1	A	272	ASP	N-CA-C	-5.67	95.68	111.00
1	A	344	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	116	ASP	CB-CA-C	5.33	121.07	110.40
1	B	94	TRP	CB-CA-C	-5.17	100.06	110.40

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	3382	0	3220	197	0
1	B	3385	0	3195	208	0
2	A	69	0	0	5	0
2	B	44	0	0	6	0
All	All	6880	0	6415	404	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 31.

The worst 5 of 404 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:108:ILE:HD12	1:A:109:ILE:N	1.45	1.31
1:B:93:GLY:N	1:B:442:LYS:HD2	1.44	1.28
1:A:108:ILE:HD12	1:A:108:ILE:C	1.49	1.24
1:A:357:PHE:CE1	1:A:361:MET:CE	2.32	1.12
1:A:447:THR:HG22	1:A:450:GLN:H	1.00	1.11

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	429/492 (87%)	405 (94%)	23 (5%)	1 (0%)	52	75
1	B	431/492 (88%)	407 (94%)	23 (5%)	1 (0%)	52	75
All	All	860/984 (87%)	812 (94%)	46 (5%)	2 (0%)	52	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	441	GLN
1	A	274	SER

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	354/417 (85%)	310 (88%)	44 (12%)	6	11
1	B	354/417 (85%)	306 (86%)	48 (14%)	5	8
All	All	708/834 (85%)	616 (87%)	92 (13%)	5	9

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	THR
1	B	103	VAL
1	B	442	LYS
1	A	456	SER
1	B	78	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	402	ASN
1	B	76	ASN
1	B	403	GLN
1	A	403	GLN
1	B	84	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 carbohydrates 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	433/492 (88%)	0.18	5 (1%) 81 83	25, 48, 75, 97	5 (1%)
1	B	435/492 (88%)	0.17	3 (0%) 89 90	27, 48, 80, 97	1 (0%)
All	All	868/984 (88%)	0.17	8 (0%) 85 88	25, 48, 76, 97	6 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	452	PHE	4.2
1	A	107	ALA	3.6
1	B	467	VAL	3.1
1	B	196	THR	3.0
1	A	196	THR	2.5

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 carbohydrates 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.