



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:45 PM GMT

PDB ID : 3UW8  
Title : Crystal Structure Analysis of the Ser305Thr Variants of KatG from *Haloarcula marismortui*  
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Deposited on : 2011-12-01  
Resolution : 2.35 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](mailto: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.

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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

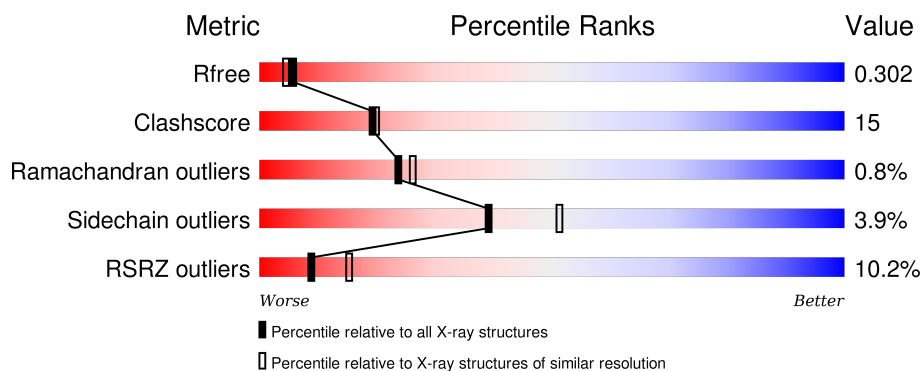
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


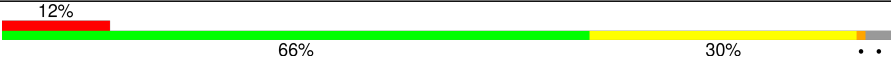
The reported resolution of this entry is 2.35 Å.

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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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  $\geq 3$ , 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	737	
1	B	737	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11563 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 Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	0	0	0
			5621	3513	945	1144	19			
1	B	714	Total	C	N	O	S	0	0	0
			5621	3513	945	1144	19			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	THR	SER	ENGINEERED MUTATION	UNP O59651
A	732	HIS	-	EXPRESSION TAG	UNP O59651
A	733	HIS	-	EXPRESSION TAG	UNP O59651
A	734	HIS	-	EXPRESSION TAG	UNP O59651
A	735	HIS	-	EXPRESSION TAG	UNP O59651
A	736	HIS	-	EXPRESSION TAG	UNP O59651
A	737	HIS	-	EXPRESSION TAG	UNP O59651
B	305	THR	SER	ENGINEERED MUTATION	UNP O59651
B	732	HIS	-	EXPRESSION TAG	UNP O59651
B	733	HIS	-	EXPRESSION TAG	UNP O59651
B	734	HIS	-	EXPRESSION TAG	UNP O59651
B	735	HIS	-	EXPRESSION TAG	UNP O59651
B	736	HIS	-	EXPRESSION TAG	UNP O59651
B	737	HIS	-	EXPRESSION TAG	UNP O59651

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

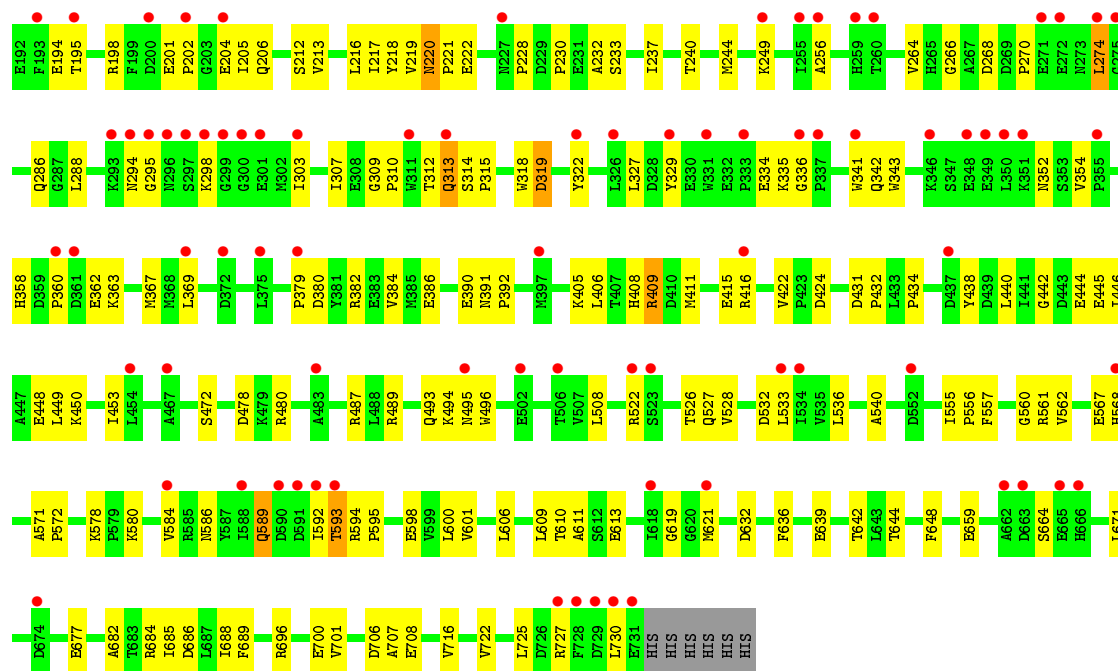


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	169	Total O 169 169	0	0
3	B	66	Total O 66 66	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	315.41Å 81.12Å 75.02Å 90.00° 99.84° 90.00°	Depositor
Resolution (Å)	24.81 – 2.35 24.81 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.81-2.35) 99.6 (24.81-2.35)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.36Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.257 , 0.309 0.253 , 0.302	Depositor DCC
$R_{free}$ test set	3920 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 77588 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11563	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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	0.45	0/5757	0.64	0/7822
1	B	0.39	0/5757	0.57	0/7822
All	All	0.42	0/11514	0.61	0/15644

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

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	5621	0	5267	173	0
1	B	5621	0	5267	167	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	169	0	0	4	0
3	B	66	0	0	4	0
All	All	11563	0	10594	330	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 15.

The worst 5 of 330 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:218:TYR:HE2	1:B:244:MET:SD	1.36	1.48
1:B:218:TYR:CE2	1:B:244:MET:SD	2.18	1.37
1:A:95:TRP:HH2	1:A:218:TYR:CE1	1.44	1.36
1:A:95:TRP:CH2	1:A:218:TYR:HE1	1.51	1.27
1:B:95:TRP:CH2	1:B:218:TYR:HE1	1.61	1.17

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	712/737 (97%)	655 (92%)	52 (7%)	5 (1%)	26	29
1	B	712/737 (97%)	651 (91%)	54 (8%)	7 (1%)	19	20
All	All	1424/1474 (97%)	1306 (92%)	106 (7%)	12 (1%)	24	26

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	GLU
1	A	299	GLY
1	A	591	ASP
1	B	22	SER
1	B	379	PRO

### 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	590/608 (97%)	565 (96%)	25 (4%)	36	46
1	B	590/608 (97%)	569 (96%)	21 (4%)	42	55
All	All	1180/1216 (97%)	1134 (96%)	46 (4%)	39	51

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	532	ASP
1	B	18	LYS
1	B	593	THR
1	A	586	ASN
1	A	667	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	HIS
1	B	227	ASN
1	B	586	ASN
1	B	220	ASN
1	B	286	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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	HEM	A	800	1	30,50,50	3.53	10 (33%)	24,82,82	10.16	16 (66%)
2	HEM	B	800	1	30,50,50	3.28	11 (36%)	24,82,82	9.67	16 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	800	1	-	0/10/54/54	0/0/8/8
2	HEM	B	800	1	-	0/10/54/54	0/0/8/8

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	HEM	C2D-C3D	-6.20	1.35	1.54
2	B	800	HEM	C2D-C3D	-6.11	1.36	1.54
2	B	800	HEM	C3B-C4B	-5.47	1.47	1.51
2	A	800	HEM	C2C-C1C	-4.61	1.43	1.52
2	A	800	HEM	C3D-C4D	-4.24	1.46	1.51

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	CAA-C2A-C1A	-13.03	112.86	127.01
2	A	800	HEM	CAA-C2A-C1A	-11.65	114.36	127.01
2	A	800	HEM	CHD-C1D-ND	-10.05	100.32	124.52
2	B	800	HEM	CHC-C4B-NB	-9.55	101.52	124.52
2	A	800	HEM	CHC-C4B-NB	-9.19	102.39	124.52

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	800	HEM	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	714/737 (96%)	0.50	55 (7%) 16 25	20, 38, 65, 93	0
1	B	714/737 (96%)	0.86	91 (12%) 5 9	26, 49, 74, 99	0
All	All	1428/1474 (96%)	0.68	146 (10%) 9 15	20, 43, 71, 99	0

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	ASN	13.2
1	B	296	ASN	12.5
1	A	298	LYS	11.4
1	A	299	GLY	10.8
1	B	730	LEU	10.6

### 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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	B	800	43/43	0.95	0.25	1.36	47,50,55,60	0
2	HEM	A	800	43/43	0.97	0.17	0.22	22,29,33,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.