



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4AE8 / pdb\_00004ae8  
Title : Crystal structure of human THEM4  
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Deposited on : 2012-01-09  
Resolution : 1.59 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

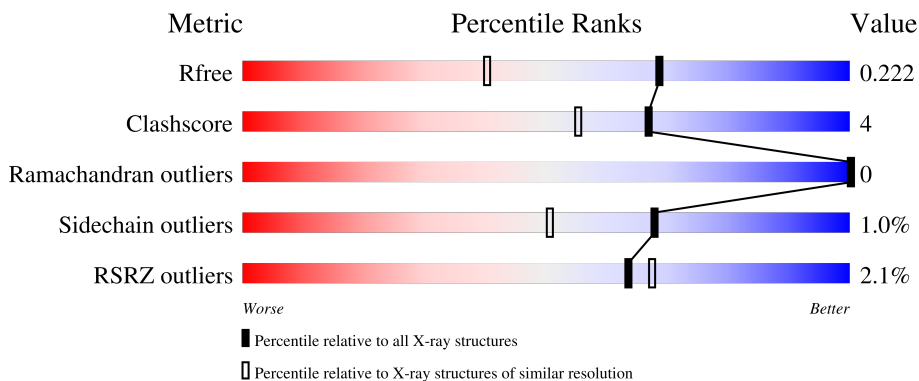
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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  $\geq 3$ , 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	211	
1	B	211	
1	C	211	
1	D	211	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6079 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 THIOESTERASE SUPERFAMILY MEMBER 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	167	Total 1338	C 857	N 222	O 244	S 15	0	3	0
1	B	166	Total 1335	C 855	N 219	O 244	S 17	0	4	0
1	C	168	Total 1337	C 856	N 221	O 244	S 16	0	2	0
1	D	165	Total 1318	C 844	N 216	O 242	S 16	0	3	0

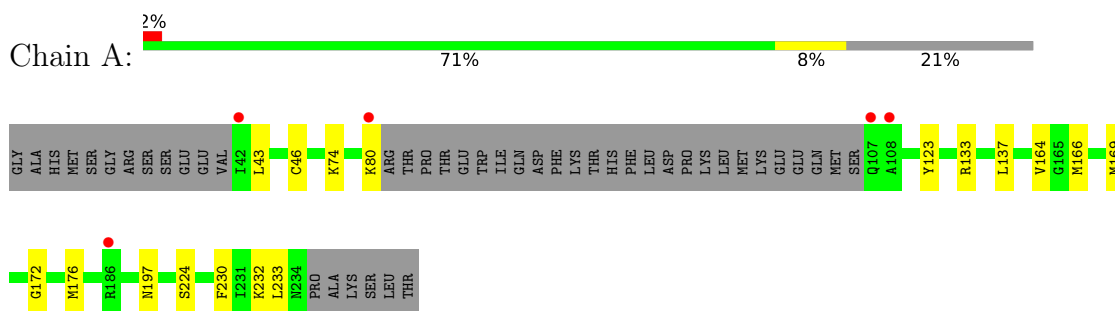
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	215	Total 215	O 215	0	0
2	B	187	Total 187	O 187	0	0
2	C	177	Total 177	O 177	0	0
2	D	172	Total 172	O 172	0	0

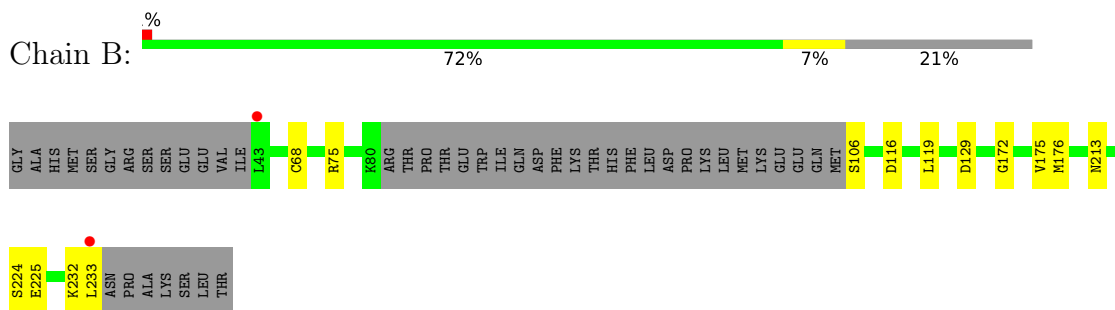
### 3 Residue-property plots [i](#)

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.

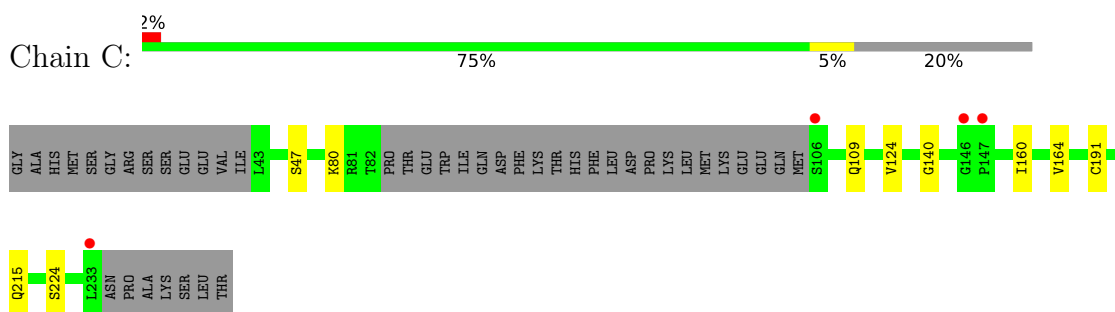
- Molecule 1: THIOESTERASE SUPERFAMILY MEMBER 4



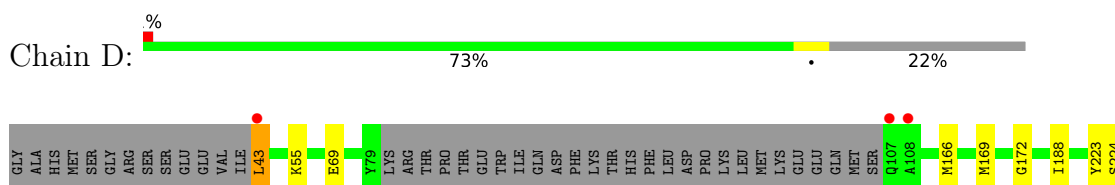
- Molecule 1: THIOESTERASE SUPERFAMILY MEMBER 4



- Molecule 1: THIOESTERASE SUPERFAMILY MEMBER 4



- Molecule 1: THIOESTERASE SUPERFAMILY MEMBER 4



K232	PRO
L233	ALA
N234	LYS
	SER
	LEU
	THR

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.54Å 58.21Å 69.68Å 89.96° 71.14° 64.60°	Depositor
Resolution (Å)	29.72 – 1.59 29.72 – 1.59	Depositor EDS
% Data completeness (in resolution range)	93.4 (29.72-1.59) 93.4 (29.72-1.59)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 1.59Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.185 , 0.223 0.184 , 0.222	Depositor DCC
$R_{free}$ test set	4114 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtrriage
Anisotropy	0.217	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.013 for h,h-k,h-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6079	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.25% 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, 0.333 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	0.43	0/1366	0.69	0/1838
1	B	0.41	0/1363	0.68	0/1833
1	C	0.39	0/1365	0.67	0/1836
1	D	0.40	0/1346	0.69	0/1812
All	All	0.41	0/5440	0.68	0/7319

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 [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	1338	0	1333	14	0
1	B	1335	0	1326	12	0
1	C	1337	0	1333	6	0
1	D	1318	0	1305	7	1
2	A	215	0	0	3	2
2	B	187	0	0	6	1
2	C	177	0	0	1	2
2	D	172	0	0	1	0
All	All	6079	0	5297	39	3

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 4.

The worst 5 of 39 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:68:CYS:SG	2:B:2051:HOH:O	2.28	0.91
1:B:129:ASP:OD1	2:B:2101:HOH:O	1.94	0.85
1:B:213[A]:ASN:OD1	1:B:225:GLU:HG2	1.91	0.69
1:D:69:GLU:OE1	2:D:2042:HOH:O	2.10	0.67
1:B:106:SER:N	2:B:2077:HOH:O	2.28	0.67

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2026:HOH:O	2:C:2049:HOH:O[1_545]	2.07	0.13
1:D:232:LYS:NZ	2:B:2173:HOH:O[1_556]	2.10	0.10
2:A:2016:HOH:O	2:C:2050:HOH:O[1_545]	2.13	0.07

## 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	166/211 (79%)	165 (99%)	1 (1%)	0	100	100
1	B	166/211 (79%)	164 (99%)	2 (1%)	0	100	100
1	C	166/211 (79%)	163 (98%)	3 (2%)	0	100	100
1	D	164/211 (78%)	162 (99%)	2 (1%)	0	100	100
All	All	662/844 (78%)	654 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	149/186 (80%)	147 (99%)	2 (1%)	61	40
1	B	149/186 (80%)	148 (99%)	1 (1%)	76	63
1	C	149/186 (80%)	148 (99%)	1 (1%)	76	63
1	D	147/186 (79%)	145 (99%)	2 (1%)	59	38
All	All	594/744 (80%)	588 (99%)	6 (1%)	68	50

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	224	SER
1	D	43	LEU
1	D	224	SER
1	A	224	SER
1	A	43	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	B	215	GLN
1	C	109	GLN
1	D	109	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, 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	167/211 (79%)	-0.10	5 (2%) 52 55	6, 15, 34, 57	3 (1%)
1	B	166/211 (78%)	-0.11	2 (1%) 76 80	7, 17, 32, 53	4 (2%)
1	C	168/211 (79%)	0.02	4 (2%) 59 63	9, 18, 37, 52	2 (1%)
1	D	165/211 (78%)	-0.13	3 (1%) 67 71	7, 16, 33, 55	3 (1%)
All	All	666/844 (78%)	-0.08	14 (2%) 63 67	6, 17, 35, 57	12 (1%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	ILE	3.8
1	D	108	ALA	3.7
1	D	43	LEU	3.5
1	D	107	GLN	3.5
1	A	80	LYS	3.0

### 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.