wwPDB X-ray Structure Validation Summary Report (i)

Apr 27, 2024 – 04:56 pm BST

PDB ID	:	4AE8
Title	:	Crystal structure of human THEM4
Authors	:	Zhuravleva, E.; Gut, H.; Hynx, D.; Marcellin, D.; Bleck, C.K.E.; Genoud, C.; Cron, P.; Keusch, J.J.; Dummler, B.; Degli Esposti, M.; Hemmings, B.A.
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

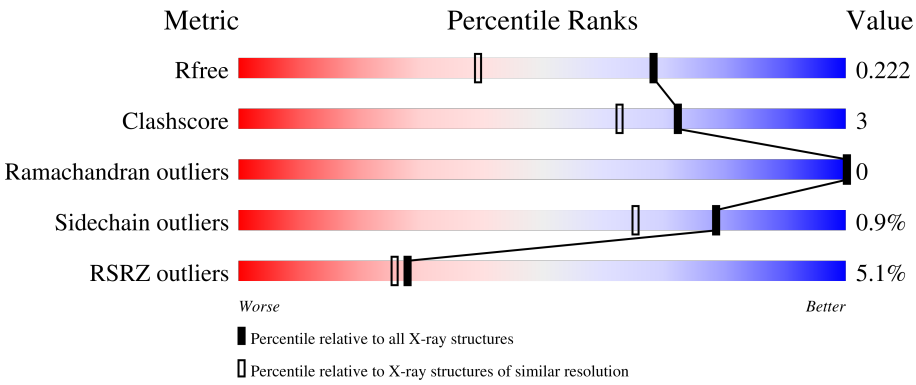
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 >=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 <=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	5% 73% 7% 21%
1	B	211	4% 71% 8% 21%
1	C	211	3% 75% 5% 20%
1	D	211	4% 73% • 22%

2 Entry composition (i)

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	1338	857	222	244	15	0	3	0
1	B	166	1335	855	219	244	17	0	4	0
1	C	168	1337	856	221	244	16	0	2	0
1	D	165	1318	844	216	242	16	0	3	0

- Molecule 2 is water.

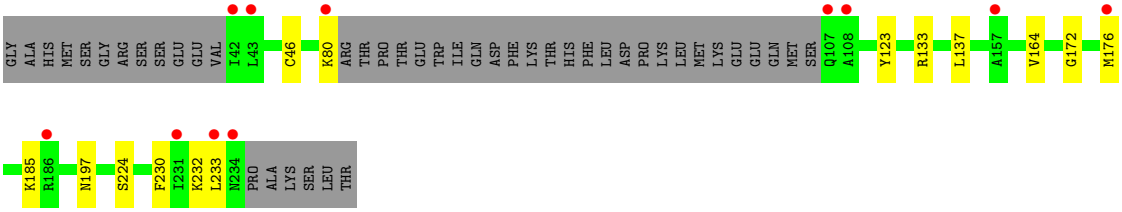
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	215	215	215	0	0
2	B	187	187	187	0	0
2	C	177	177	177	0	0
2	D	172	172	172	0	0

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.

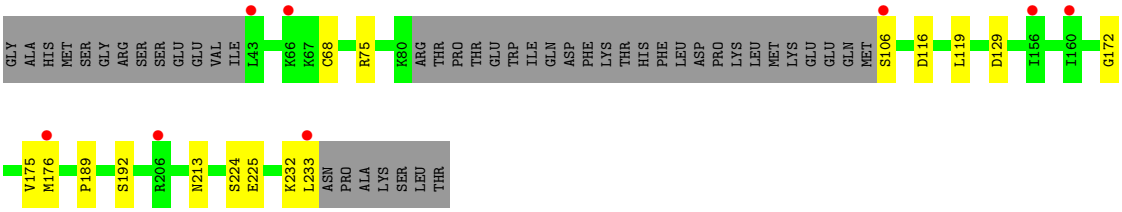
• Molecule 1: THIOESTERASE SUPERFAMILY MEMBER 4

Chain A:



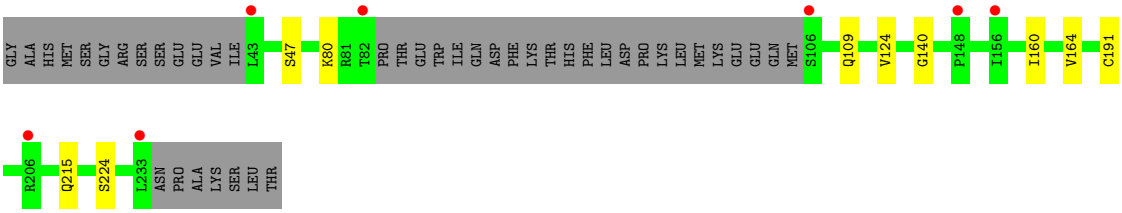
• Molecule 1: THIOESTERASE SUPERFAMILY MEMBER 4

Chain B:



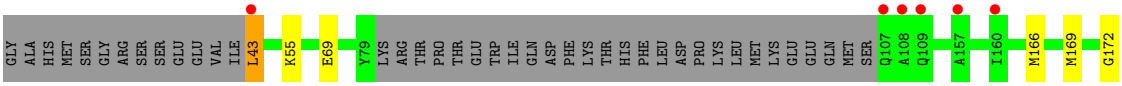
• Molecule 1: THIOESTERASE SUPERFAMILY MEMBER 4

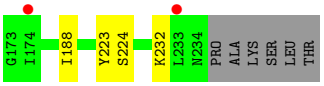
Chain C:



• Molecule 1: THIOESTERASE SUPERFAMILY MEMBER 4

Chain D:




G173
I174
I188
Y223
S224
K232
L233
N234
PRO
ALA
LYS
SER
LEU
THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.41 (at 1.59Å)	Xtriage
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^2)	15.0	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6079	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage'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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.36	0/1366	0.52	0/1838
1	B	0.35	0/1363	0.50	0/1833
1	C	0.34	0/1365	0.48	0/1836
1	D	0.35	0/1346	0.51	0/1812
All	All	0.35	0/5440	0.51	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	12	0
1	B	1335	0	1326	12	0
1	C	1337	0	1333	6	0
1	D	1318	0	1305	6	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	36	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 3.

The worst 5 of 36 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%)	148 (99%)	1 (1%)	84	73
1	B	149/186 (80%)	148 (99%)	1 (1%)	84	73
1	C	149/186 (80%)	148 (99%)	1 (1%)	84	73
1	D	147/186 (79%)	145 (99%)	2 (1%)	67	47
All	All	594/744 (80%)	589 (99%)	5 (1%)	78	70

All (5) residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	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 monosaccharides 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	167/211 (79%)	0.46	11 (6%)	18	17	8, 15, 34, 57	0
1	B	166/211 (78%)	0.39	8 (4%)	30	28	9, 17, 32, 53	0
1	C	168/211 (79%)	0.42	7 (4%)	36	33	10, 19, 37, 52	0
1	D	165/211 (78%)	0.37	8 (4%)	30	28	10, 16, 33, 55	0
All	All	666/844 (78%)	0.41	34 (5%)	28	26	8, 17, 35, 57	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	ILE	11.3
1	D	107	GLN	7.5
1	A	43	LEU	6.6
1	B	233	LEU	6.3
1	D	108	ALA	5.9

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 monosaccharides 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.