



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:39 am GMT

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 Full wwPDB X-ray Structure Validation 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

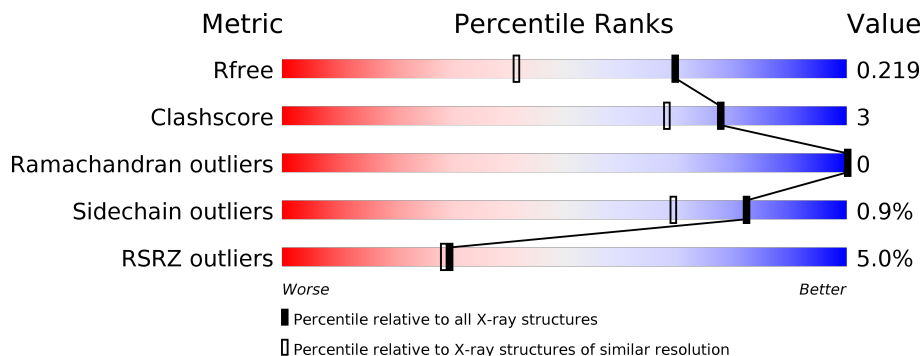
1 Overall quality at a glance

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}	100719	2696 (1.60-1.60)
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (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 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	211	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>7%</div> <div>21%</div> </div> </div>
1	B	211	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>8%</div> <div>21%</div> </div> </div>
1	C	211	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>5%</div> <div>20%</div> </div> </div>
1	D	211	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>•</div> <div>22%</div> </div> </div>

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.

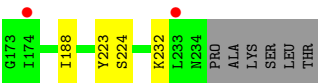
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	3	0
			1338	857	222	244	15			
1	B	166	Total	C	N	O	S	0	4	0
			1335	855	219	244	17			
1	C	168	Total	C	N	O	S	0	2	0
			1337	856	221	244	16			
1	D	165	Total	C	N	O	S	0	3	0
			1318	844	216	242	16			

- Molecule 2 is water.

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

● Molecule 1: THIOESTERASE SUPERFAMILY MEMBER 4





4 Data and refinement statistics

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) 89.4 (29.72-1.59)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.59Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.185 , 0.223 0.180 , 0.219	Depositor DCC
R_{free} test set	4115 reflections (4.93%)	DCC
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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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	0.36	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.

All (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
1:C:80:LYS:HE3	1:C:109:GLN:NE2	2.12	0.64
1:B:176:MET:HG2	1:B:233:LEU:HD11	1.83	0.61
2:B:2080:HOH:O	1:D:55:LYS:NZ	2.37	0.58
1:A:46:CYS:SG	1:A:80:LYS:HE2	2.47	0.54
1:A:133[A]:ARG:NH2	2:A:2126:HOH:O	2.41	0.53
1:C:140:GLY:O	1:C:191:CYS:HA	2.12	0.50
1:D:172:GLY:O	1:D:232:LYS:NZ	2.40	0.50
1:D:43:LEU:O	1:D:43:LEU:HD13	2.11	0.49
1:A:176:MET:CG	1:A:233:LEU:HD11	2.42	0.49
1:A:176:MET:HG2	1:A:233:LEU:HD11	1.94	0.48
1:B:175:VAL:HG12	1:B:232:LYS:HA	1.95	0.47
1:A:133[A]:ARG:NH1	1:A:197:ASN:OD1	2.47	0.47
1:C:215:GLN:NE2	2:C:2165:HOH:O	2.44	0.45
1:B:75:ARG:N	2:B:2051:HOH:O	2.43	0.45
1:A:185:LYS:NZ	2:A:2177:HOH:O	2.46	0.45
1:C:80:LYS:HE3	1:C:109:GLN:HE22	1.83	0.43
1:A:172:GLY:O	1:A:232:LYS:NZ	2.46	0.43
1:B:213[A]:ASN:CG	2:B:2173:HOH:O	2.57	0.43
1:A:133[A]:ARG:CZ	2:A:2126:HOH:O	2.67	0.42
1:C:47:SER:HB3	1:C:124:VAL:HG23	2.02	0.42
1:D:166:MET:SD	1:D:169[A]:MET:CE	3.07	0.42
1:B:172:GLY:O	1:B:232:LYS:HE2	2.20	0.42
1:C:160:ILE:O	1:C:164:VAL:HG22	2.20	0.42
1:B:189:PRO:HB2	1:B:192:SER:HG	1.85	0.42
1:A:46:CYS:SG	1:A:80:LYS:HG2	2.60	0.41
1:B:213[B]:ASN:O	1:B:213[B]:ASN:OD1	2.38	0.41
1:D:188:ILE:HG12	1:D:223:TYR:CD1	2.55	0.41
1:A:164:VAL:HG23	1:A:230:PHE:CE1	2.55	0.41
1:B:116:ASP:HB2	1:B:119:LEU:HD12	2.02	0.41
1:A:176:MET:HG2	1:A:233:LEU:CD1	2.51	0.40
1:A:123:TYR:HA	1:A:137:LEU:O	2.22	0.40

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%)	87	77
1	B	149/186 (80%)	148 (99%)	1 (1%)	87	77
1	C	149/186 (80%)	148 (99%)	1 (1%)	87	77
1	D	147/186 (79%)	145 (99%)	2 (1%)	71	52
All	All	594/744 (80%)	589 (99%)	5 (1%)	82	73

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

Some 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 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	0.45	11 (6%) 19 18	8, 15, 34, 57	0
1	B	166/211 (78%)	0.38	7 (4%) 37 35	9, 17, 32, 53	0
1	C	168/211 (79%)	0.40	7 (4%) 37 35	10, 19, 37, 52	0
1	D	165/211 (78%)	0.36	8 (4%) 31 30	10, 16, 33, 55	0
All	All	666/844 (78%)	0.40	33 (4%) 30 28	8, 17, 35, 57	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	ILE	11.4
1	D	107	GLN	7.4
1	A	43	LEU	6.6
1	B	233	LEU	6.3
1	D	108	ALA	5.9
1	C	233	LEU	5.8
1	A	80	LYS	5.7
1	D	43	LEU	5.4
1	B	43	LEU	4.9
1	A	108	ALA	4.8
1	A	107	GLN	4.2
1	C	106	SER	3.2
1	C	148	PRO	2.8
1	B	206	ARG	2.7
1	C	43	LEU	2.7
1	A	176	MET	2.5
1	C	156	ILE	2.5
1	C	206	ARG	2.4
1	D	109	GLN	2.4
1	B	156	ILE	2.3
1	D	233	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	231	ILE	2.3
1	B	66	LYS	2.3
1	D	160	ILE	2.3
1	D	174	ILE	2.3
1	A	233	LEU	2.2
1	C	82	THR	2.2
1	B	106	SER	2.2
1	A	157	ALA	2.1
1	A	186	ARG	2.1
1	D	157	ALA	2.1
1	A	234	ASN	2.0
1	B	160	ILE	2.0

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 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.