



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:27 am GMT

PDB ID : 3TEC
Title : CALCIUM BINDING TO THERMITASE. CRYSTALLOGRAPHIC STUDIES OF THERMITASE AT 0, 5 AND 100 MM CALCIUM
Authors : Gros, P.; Kalk, K.H.; Hol, W.G.J.
Deposited on : 1990-10-26
Resolution : 2.00 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

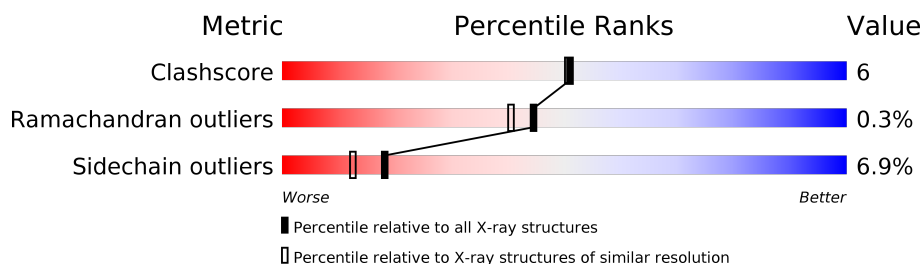
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	279	 75% 20% . .
2	I	70	 63% 19% 7% . 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2659 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 THERMITASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	279	Total	C	N	O	S	0	0	0
			2004	1242	351	409	2			

- Molecule 2 is a protein called EGLIN C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	63	Total	C	N	O	0	0	0
			522	339	89	94			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	3	Total	Ca	0	0
			3	3		

- Molecule 4 is water.

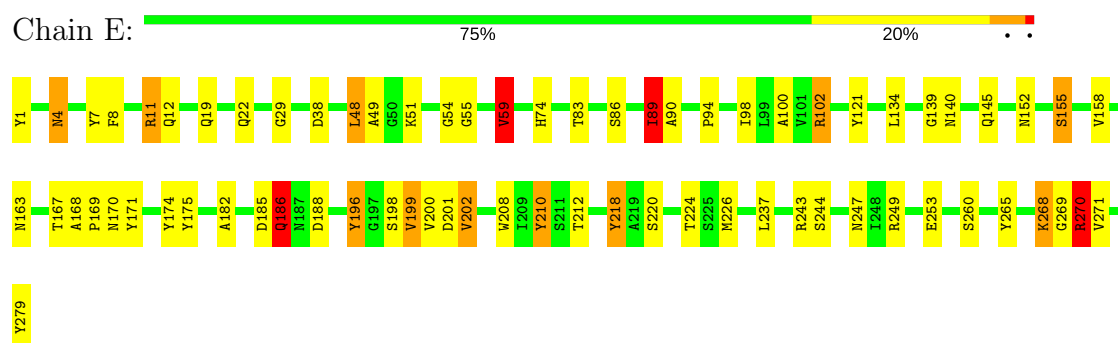
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	108	Total	O	0	0
			108	108		
4	I	22	Total	O	0	0
			22	22		

3 Residue-property plots [i](#)

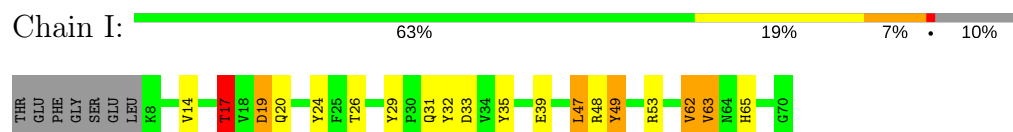
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: THERMITASE



• Molecule 2: EGLIN C



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.24Å 71.77Å 88.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GROMOS	Depositor
R, R_{free}	0.168 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2659	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	E	0.98	1/2049 (0.0%)	1.64	37/2805 (1.3%)
2	I	1.00	0/540	1.75	14/738 (1.9%)
All	All	0.98	1/2589 (0.0%)	1.67	51/3543 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	8
2	I	0	4
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	199	VAL	CA-CB	5.13	1.65	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	270	ARG	NE-CZ-NH1	18.30	129.45	120.30
1	E	270	ARG	NE-CZ-NH2	-13.10	113.75	120.30
1	E	175	TYR	CB-CG-CD2	-12.55	113.47	121.00
1	E	199	VAL	CG1-CB-CG2	-11.65	92.26	110.90
1	E	196	TYR	CB-CG-CD1	-10.23	114.86	121.00
2	I	35	TYR	CB-CG-CD1	-9.88	115.07	121.00
2	I	53	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	E	89	ILE	CA-CB-CG2	9.42	129.74	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	199	VAL	CA-CB-CG2	8.38	123.47	110.90
1	E	199	VAL	CA-CB-CG1	7.95	122.82	110.90
2	I	48	ARG	NE-CZ-NH2	7.69	124.15	120.30
1	E	270	ARG	CD-NE-CZ	7.48	134.08	123.60
1	E	102	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	E	202	VAL	CA-CB-CG1	7.24	121.76	110.90
1	E	279	TYR	CB-CG-CD1	-7.07	116.76	121.00
1	E	140	ASN	N-CA-CB	-6.74	98.47	110.60
1	E	218	TYR	CB-CG-CD1	-6.74	116.96	121.00
2	I	62	VAL	CA-CB-CG2	6.70	120.94	110.90
1	E	171	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	E	59	VAL	CG1-CB-CG2	6.47	121.25	110.90
1	E	265	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	E	185	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	E	174	TYR	CB-CG-CD1	-6.28	117.23	121.00
1	E	11	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	E	155	SER	CB-CA-C	6.23	121.94	110.10
2	I	24	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	E	48	LEU	CB-CG-CD1	6.20	121.54	111.00
2	I	17	THR	N-CA-CB	-6.09	98.72	110.30
1	E	210	TYR	CB-CG-CD2	-6.06	117.37	121.00
1	E	59	VAL	CA-CB-CG2	5.98	119.87	110.90
1	E	244	SER	N-CA-CB	-5.93	101.60	110.50
2	I	63	VAL	CA-CB-CG1	5.92	119.78	110.90
2	I	35	TYR	CG-CD1-CE1	-5.91	116.58	121.30
2	I	14	VAL	CG1-CB-CG2	-5.80	101.61	110.90
1	E	271	VAL	CG1-CB-CG2	-5.74	101.72	110.90
2	I	19	ASP	CB-CG-OD2	-5.73	113.15	118.30
1	E	1	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	E	186	GLN	CB-CA-C	-5.72	98.95	110.40
1	E	152	ASN	CA-CB-CG	-5.71	100.85	113.40
1	E	7	TYR	CB-CG-CD1	-5.62	117.63	121.00
2	I	49	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	E	121	TYR	CB-CG-CD1	-5.51	117.69	121.00
2	I	35	TYR	CD1-CG-CD2	5.49	123.94	117.90
1	E	202	VAL	N-CA-CB	-5.49	99.43	111.50
1	E	158	VAL	CA-CB-CG1	-5.47	102.69	110.90
2	I	33	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	E	270	ARG	NH1-CZ-NH2	-5.24	113.64	119.40
2	I	47	LEU	CA-CB-CG	-5.08	103.63	115.30
1	E	198	SER	C-N-CA	5.04	134.31	121.70
1	E	249	ARG	NE-CZ-NH1	5.03	122.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	260	SER	CB-CA-C	5.03	119.65	110.10

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	11	ARG	Sidechain
1	E	139	GLY	Mainchain
1	E	155	SER	Mainchain
1	E	218	TYR	Sidechain
1	E	269	GLY	Mainchain
1	E	270	ARG	Sidechain
1	E	29	GLY	Mainchain
1	E	54	GLY	Mainchain
2	I	26	THR	Mainchain
2	I	29	TYR	Sidechain
2	I	32	TYR	Sidechain
2	I	49	TYR	Sidechain

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	E	2004	0	1909	29	0
2	I	522	0	498	3	0
3	E	3	0	0	0	0
4	E	108	0	0	1	0
4	I	22	0	0	1	0
All	All	2659	0	2407	32	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 6.

All (32) 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:E:12:GLN:HE22	1:E:90:ALA:H	1.30	0.80
1:E:4:ASN:HD21	1:E:86:SER:H	1.29	0.78
1:E:243:ARG:HH21	1:E:247:ASN:HD21	1.35	0.72
2:I:17:THR:HG21	4:I:87:HOH:O	1.89	0.70
2:I:17:THR:HG22	2:I:20:GLN:H	1.56	0.70
1:E:4:ASN:ND2	1:E:86:SER:H	1.90	0.68
1:E:186:GLN:NE2	1:E:186:GLN:H	1.91	0.67
1:E:19:GLN:HE21	1:E:22:GLN:NE2	1.94	0.66
1:E:186:GLN:HE21	1:E:186:GLN:H	1.48	0.61
1:E:12:GLN:NE2	1:E:90:ALA:H	1.98	0.60
1:E:163:ASN:HD21	1:E:224:THR:H	1.49	0.59
1:E:8:PHE:HA	1:E:12:GLN:HE21	1.70	0.56
1:E:253:GLU:HB3	1:E:268:LYS:HG2	1.87	0.55
1:E:188:ASP:OD2	1:E:270:ARG:HD3	2.08	0.54
1:E:4:ASN:HD22	1:E:4:ASN:C	2.10	0.54
1:E:182:ALA:HB2	1:E:200:VAL:HG11	1.89	0.54
1:E:89:ILE:HD11	1:E:210:TYR:CD1	2.45	0.52
1:E:55:GLY:HA3	1:E:100:ALA:O	2.11	0.51
1:E:208:TRP:HE3	1:E:220:SER:OG	1.95	0.50
1:E:49:ALA:HA	4:E:411:HOH:O	2.11	0.50
2:I:39:GLU:OE2	2:I:65:HIS:NE2	2.46	0.49
1:E:243:ARG:HB3	1:E:247:ASN:HD22	1.78	0.48
1:E:51:LYS:HB3	1:E:98:ILE:HD12	1.99	0.45
1:E:243:ARG:HH21	1:E:247:ASN:ND2	2.09	0.44
1:E:59:VAL:HG22	1:E:102:ARG:NH1	2.33	0.43
1:E:83:THR:HB	1:E:94:PRO:HB3	2.00	0.43
1:E:201:ASP:O	1:E:268:LYS:HB2	2.19	0.42
1:E:74:HIS:HA	1:E:212:THR:O	2.20	0.42
1:E:167:THR:HA	1:E:196:TYR:O	2.20	0.41
1:E:163:ASN:ND2	1:E:224:THR:H	2.16	0.41
1:E:168:ALA:HA	1:E:169:PRO:HD3	1.96	0.40
1:E:134:LEU:HD12	1:E:134:LEU:C	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	E	277/279 (99%)	268 (97%)	8 (3%)	1 (0%)	38	33
2	I	61/70 (87%)	60 (98%)	1 (2%)	0	100	100
All	All	338/349 (97%)	328 (97%)	9 (3%)	1 (0%)	44	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	38	ASP

5.3.2 Protein sidechains ⓘ

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	E	202/202 (100%)	190 (94%)	12 (6%)	23	17
2	I	58/64 (91%)	52 (90%)	6 (10%)	8	4
All	All	260/266 (98%)	242 (93%)	18 (7%)	18	12

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	ASN
1	E	48	LEU
1	E	59	VAL
1	E	89	ILE
1	E	145	GLN
1	E	170	ASN
1	E	186	GLN
1	E	199	VAL
1	E	202	VAL
1	E	226	MET
1	E	237	LEU
1	E	268	LYS

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Mol	Chain	Res	Type
2	I	17	THR
2	I	19	ASP
2	I	31	GLN
2	I	47	LEU
2	I	62	VAL
2	I	63	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	4	ASN
1	E	12	GLN
1	E	22	GLN
1	E	117	ASN
1	E	148	ASN
1	E	152	ASN
1	E	163	ASN
1	E	170	ASN
1	E	177	ASN
1	E	186	GLN
1	E	247	ASN

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 ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.