



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:20 AM UTC

PDB ID : 3TEC / pdb\_00003tec  
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](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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

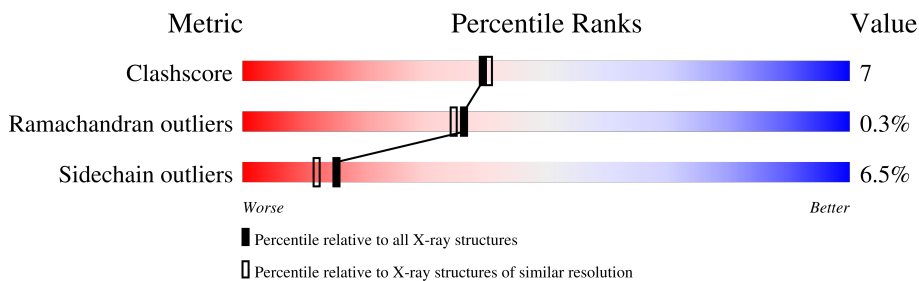
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	279	 75% 20% . .
2	I	70	 67% 17% . . 10%

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	E	279	2004	1242	351	409	2	0	0	0

- Molecule 2 is a protein called EGLIN C.

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is water.

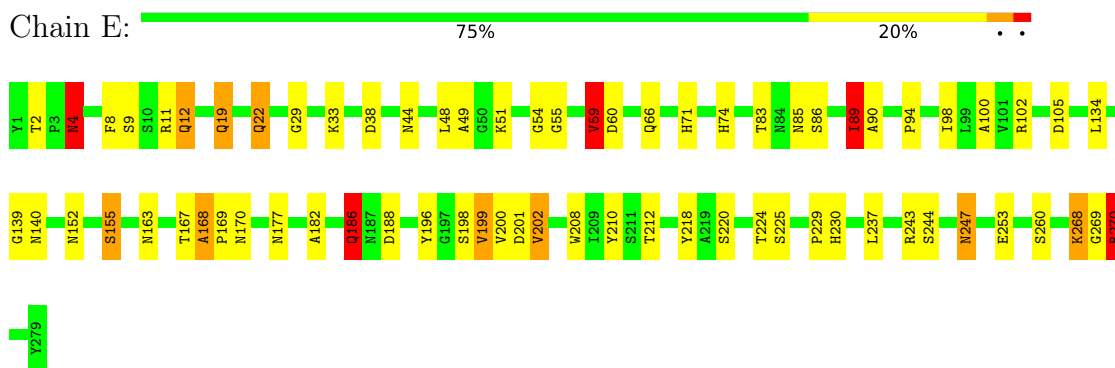
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	108	108	108	0	0
4	I	22	22	22	0	0

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

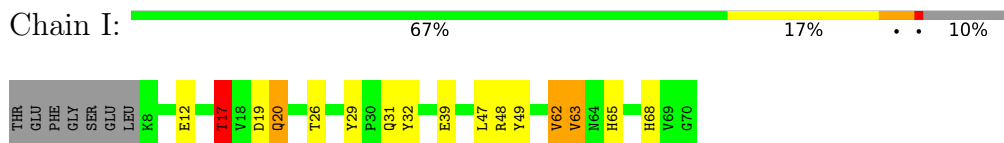
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	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.	Xtrriage
Total number of atoms	2659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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	1.25	6/2049 (0.3%)	1.84	43/2805 (1.5%)
2	I	1.22	0/540	1.84	9/738 (1.2%)
All	All	1.24	6/2589 (0.2%)	1.84	52/3543 (1.5%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	199	VAL	CA-CB	8.13	1.65	1.54
1	E	66	GLN	CD-NE2	-5.78	1.21	1.33
1	E	85	ASN	CG-ND2	-5.77	1.21	1.33
1	E	230	HIS	CG-ND1	-5.38	1.32	1.38
1	E	71	HIS	CG-ND1	-5.27	1.32	1.38
1	E	199	VAL	N-CA	5.07	1.52	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	152	ASN	CA-CB-CG	-11.75	100.85	112.60
1	E	89	ILE	CA-CB-CG2	11.32	129.74	110.50
1	E	89	ILE	N-CA-CB	-9.92	101.03	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	66	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	E	60	ASP	CA-CB-CG	8.56	121.17	112.60
1	E	199	VAL	CG1-CB-CG2	-8.43	92.26	110.80
2	I	20	GLN	OE1-CD-NE2	-8.24	114.36	122.60
2	I	17	THR	N-CA-CB	-8.07	98.72	110.26
1	E	270	ARG	NE-CZ-NH1	7.95	129.45	121.50
1	E	199	VAL	CA-CB-CG2	7.69	123.47	110.40
1	E	199	VAL	CA-CB-CG1	7.30	122.82	110.40
1	E	155	SER	CB-CA-C	7.17	121.94	110.19
1	E	198	SER	CA-C-O	-7.13	111.77	119.97
1	E	140	ASN	N-CA-CB	-7.11	98.47	110.49
1	E	202	VAL	N-CA-CB	-6.99	99.43	112.36
1	E	270	ARG	CD-NE-CZ	6.91	134.08	124.40
1	E	198	SER	CA-C-N	6.85	134.31	121.97
1	E	198	SER	C-N-CA	6.85	134.31	121.97
2	I	63	VAL	CB-CA-C	6.79	118.56	111.23
1	E	202	VAL	CA-CB-CG1	6.68	121.76	110.40
1	E	19	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	E	198	SER	O-C-N	6.48	130.24	122.27
1	E	155	SER	O-C-N	-6.47	115.63	123.27
1	E	59	VAL	N-CA-C	6.27	116.90	110.82
2	I	62	VAL	CA-CB-CG2	6.20	120.94	110.40
1	E	244	SER	N-CA-CB	-6.13	101.60	110.36
1	E	270	ARG	NE-CZ-NH2	-6.05	113.75	119.20
1	E	152	ASN	N-CA-C	6.03	118.65	111.71
1	E	247	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	E	260	SER	CB-CA-C	5.98	119.65	109.72
1	E	229	PRO	N-CA-CB	5.93	108.98	103.41
1	E	105	ASP	CA-CB-CG	5.88	118.48	112.60
1	E	9	SER	CA-CB-OG	-5.68	99.73	111.10
2	I	12	GLU	N-CA-C	5.67	119.29	112.38
1	E	59	VAL	CA-CB-CG2	5.57	119.87	110.40
2	I	63	VAL	CA-CB-CG1	5.52	119.78	110.40
2	I	48	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	E	85	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	E	186	GLN	CB-CA-C	-5.43	98.95	110.31
2	I	68	HIS	CB-CG-CD2	-5.35	124.25	131.20
2	I	68	HIS	CA-CB-CG	-5.27	108.53	113.80
1	E	2	THR	O-C-N	5.25	125.78	121.31
1	E	168	ALA	CA-C-N	5.24	125.17	119.78
1	E	168	ALA	C-N-CA	5.24	125.17	119.78
1	E	89	ILE	O-C-N	5.20	127.53	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	177	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	E	44	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	E	4	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	E	2	THR	CA-C-O	-5.13	115.51	119.46
1	E	225	SER	CB-CA-C	-5.11	102.31	110.79
1	E	12	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	E	22	GLN	OE1-CD-NE2	-5.01	117.59	122.60

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 [\(i\)](#)

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	E	2004	0	1909	30	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	33	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 7.

All (33) 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:208:TRP:HE3	1:E:220:SER:HG	1.39	0.68
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:H	1:E:186:GLN:HE21	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:4:ASN:C	1:E:4:ASN:HD22	2.10	0.58
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: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: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:134:LEU:HD12	1:E:134:LEU:C	2.42	0.45
1:E:208:TRP:HE3	1:E:220:SER:OG	1.95	0.44
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

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	E	277/279 (99%)	268 (97%)	8 (3%)	1 (0%)	30	27
2	I	61/70 (87%)	60 (98%)	1 (2%)	0	100	100
All	All	338/349 (97%)	328 (97%)	9 (3%)	1 (0%)	36	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	38	ASP

### 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	E	202/202 (100%)	191 (95%)	11 (5%)	20	17
2	I	58/64 (91%)	52 (90%)	6 (10%)	7	4
All	All	260/266 (98%)	243 (94%)	17 (6%)	15	12

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	ASN
1	E	33	LYS
1	E	48	LEU
1	E	59	VAL
1	E	89	ILE

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Mol	Chain	Res	Type
1	E	170	ASN
1	E	186	GLN
1	E	199	VAL
1	E	202	VAL
1	E	237	LEU
1	E	268	LYS
2	I	17	THR
2	I	19	ASP
2	I	31	GLN
2	I	47	LEU
2	I	62	VAL
2	I	63	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) 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	177	ASN
1	E	186	GLN
1	E	247	ASN

### 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](#)

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.