



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:22 AM UTC

PDB ID : 2TEC / pdb_00002tec
Title : MOLECULAR DYNAMICS REFINEMENT OF A THERMITASE-EGLIN-C COMPLEX AT 1.98 ANGSTROMS RESOLUTION AND COMPARISON OF TWO CRYSTAL FORMS THAT DIFFER IN CALCIUM CONTENT
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Deposited on : 1990-10-26
Resolution : 1.98 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

<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>.

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

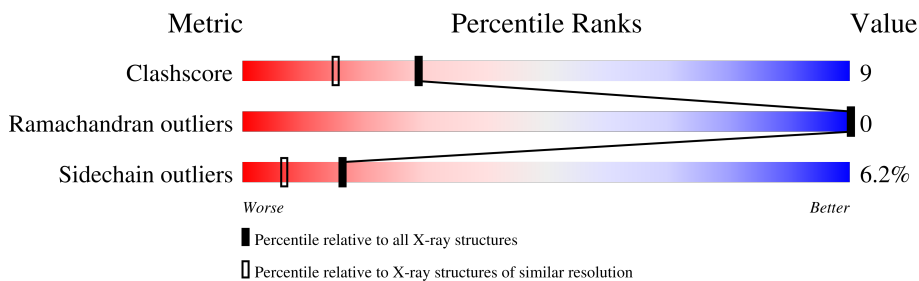
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	279	
2	I	70	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2753 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.

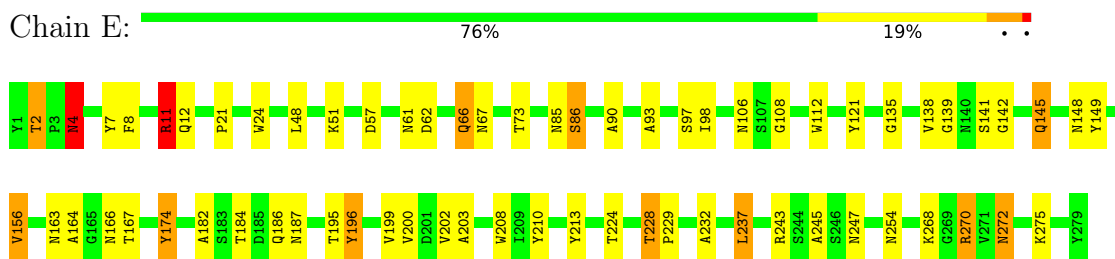
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	166	166	166	0	0
4	I	58	58	58	0	0

3 Residue-property plots

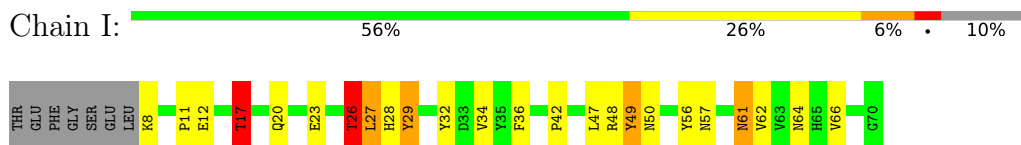
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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, α , β , γ	49.06Å 67.23Å 90.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.98	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.98)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GROMOS	Depositor
R, R_{free}	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2753	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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	1.21	1/2049 (0.0%)	1.65	24/2805 (0.9%)
2	I	1.19	0/540	1.74	5/738 (0.7%)
All	All	1.21	1/2589 (0.0%)	1.67	29/3543 (0.8%)

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	17
2	I	0	7
All	All	0	24

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	85	ASN	CG-ND2	-5.46	1.21	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4	ASN	OD1-CG-ND2	-10.82	111.78	122.60
1	E	145	GLN	CB-CA-C	-9.43	95.72	110.81
2	I	17	THR	N-CA-CB	-7.87	99.00	110.26
1	E	272	ASN	OD1-CG-ND2	-7.83	114.77	122.60
1	E	138	VAL	O-C-N	7.80	131.69	123.26
1	E	2	THR	CB-CA-C	7.24	118.10	109.85
1	E	85	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	E	145	GLN	N-CA-CB	6.38	119.45	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	11	ARG	NH1-CZ-NH2	-6.09	111.38	119.30
2	I	17	THR	CA-CB-CG2	6.06	120.81	110.50
2	I	61	ASN	CA-CB-CG	-6.06	106.54	112.60
1	E	270	ARG	CD-NE-CZ	5.97	132.76	124.40
1	E	97	SER	CB-CA-C	5.92	119.57	109.80
1	E	135	GLY	CA-C-N	5.78	126.95	121.46
1	E	135	GLY	C-N-CA	5.78	126.95	121.46
1	E	254	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	E	228	THR	CA-C-N	5.67	125.34	119.56
1	E	228	THR	C-N-CA	5.67	125.34	119.56
1	E	202	VAL	N-CA-CB	-5.55	102.10	112.36
1	E	237	LEU	N-CA-CB	-5.54	101.69	109.94
1	E	142	GLY	CA-C-O	5.35	126.26	120.75
1	E	270	ARG	NE-CZ-NH2	-5.29	114.44	119.20
2	I	28	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	E	93	ALA	CA-C-N	5.15	125.44	119.47
1	E	93	ALA	C-N-CA	5.15	125.44	119.47
1	E	97	SER	N-CA-CB	-5.12	102.57	110.56
2	I	50	ASN	N-CA-CB	-5.11	102.81	110.73
1	E	202	VAL	CB-CA-C	5.09	118.90	110.30
1	E	270	ARG	NE-CZ-NH1	5.04	126.54	121.50

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	108	GLY	Mainchain
1	E	11	ARG	Sidechain
1	E	121	TYR	Sidechain
1	E	139	GLY	Mainchain
1	E	148	ASN	Mainchain
1	E	149	TYR	Sidechain
1	E	174	TYR	Sidechain
1	E	187	ASN	Mainchain
1	E	195	THR	Mainchain
1	E	196	TYR	Sidechain
1	E	210	TYR	Sidechain
1	E	213	TYR	Sidechain
1	E	232	ALA	Mainchain
1	E	270	ARG	Sidechain
1	E	272	ASN	Sidechain
1	E	57	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	E	7	TYR	Sidechain
2	I	26	THR	Mainchain
2	I	29	TYR	Sidechain
2	I	36	PHE	Sidechain
2	I	47	LEU	Mainchain
2	I	48	ARG	Sidechain
2	I	49	TYR	Sidechain
2	I	56	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	1908	35	0
2	I	522	0	498	11	0
3	E	3	0	0	0	0
4	E	166	0	0	10	1
4	I	58	0	0	2	0
All	All	2753	0	2406	43	1

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 9.

All (43) 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:11:ARG:HH11	1:E:11:ARG:HB3	1.48	0.78
2:I:17:THR:HG22	2:I:20:GLN:H	1.47	0.78
1:E:12:GLN:HE22	1:E:90:ALA:H	1.32	0.76
1:E:66:GLN:HE21	1:E:66:GLN:H	1.34	0.76
1:E:156:VAL:HB	4:E:497:HOH:O	1.87	0.74
1:E:163:ASN:HD21	1:E:224:THR:H	1.36	0.72
1:E:186:GLN:HG2	4:E:433:HOH:O	1.96	0.64
1:E:141:SER:O	1:E:145:GLN:HG2	1.98	0.62
1:E:61:ASN:HB3	4:E:347:HOH:O	2.01	0.61
1:E:174:TYR:HE2	1:E:199:VAL:HG11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:ASN:HD21	1:E:86:SER:H	1.48	0.61
1:E:243:ARG:HH21	1:E:247:ASN:HD21	1.48	0.60
1:E:174:TYR:CE2	1:E:199:VAL:HG11	2.41	0.55
2:I:12:GLU:HB2	4:I:108:HOH:O	2.08	0.53
1:E:164:ALA:HB3	4:E:449:HOH:O	2.09	0.52
1:E:12:GLN:NE2	1:E:90:ALA:H	2.07	0.48
2:I:57:ASN:HB2	2:I:64:ASN:ND2	2.28	0.48
1:E:112:TRP:HD1	4:E:493:HOH:O	1.97	0.48
1:E:8:PHE:HA	1:E:12:GLN:HE21	1.79	0.48
1:E:243:ARG:HH21	1:E:247:ASN:ND2	2.11	0.48
1:E:66:GLN:H	1:E:66:GLN:NE2	2.06	0.47
1:E:51:LYS:HB3	1:E:98:ILE:HD12	1.96	0.47
1:E:106:ASN:HB2	4:E:364:HOH:O	2.14	0.46
2:I:23:GLU:HG2	2:I:27:LEU:HD22	1.96	0.46
1:E:182:ALA:HB2	1:E:200:VAL:HG11	1.98	0.46
1:E:275:LYS:HG2	4:E:444:HOH:O	2.17	0.45
1:E:112:TRP:CZ3	2:I:42:PRO:HB3	2.52	0.45
1:E:21:PRO:HA	1:E:24:TRP:CE3	2.51	0.44
1:E:166:ASN:HB2	4:E:473:HOH:O	2.17	0.44
1:E:4:ASN:ND2	1:E:86:SER:H	2.15	0.43
1:E:245:ALA:HA	4:E:497:HOH:O	2.18	0.43
1:E:62:ASP:HB2	4:E:346:HOH:O	2.19	0.42
1:E:184:THR:HG23	1:E:203:ALA:HB1	2.01	0.42
1:E:208:TRP:CH2	2:I:49:TYR:HE1	2.37	0.42
1:E:208:TRP:HH2	2:I:49:TYR:HE1	1.66	0.42
2:I:29:TYR:HB3	2:I:32:TYR:HD1	1.85	0.42
1:E:67:ASN:ND2	1:E:73:THR:H	2.18	0.41
2:I:11:PRO:HA	2:I:66:VAL:HG13	2.03	0.41
2:I:23:GLU:O	2:I:27:LEU:HB2	2.21	0.41
1:E:228:THR:HB	1:E:229:PRO:HD3	2.02	0.41
1:E:4:ASN:HD22	1:E:4:ASN:C	2.29	0.40
1:E:167:THR:HA	1:E:196:TYR:O	2.21	0.40
2:I:26:THR:HG22	4:I:78:HOH:O	2.20	0.40

All (1) 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)
4:E:416:HOH:O	4:E:424:HOH:O[3_655]	2.02	0.18

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%)	9 (3%)	0	100	100
2	I	61/70 (87%)	60 (98%)	1 (2%)	0	100	100
All	All	338/349 (97%)	328 (97%)	10 (3%)	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	E	202/202 (100%)	193 (96%)	9 (4%)	24	13
2	I	58/64 (91%)	51 (88%)	7 (12%)	5	1
All	All	260/266 (98%)	244 (94%)	16 (6%)	16	7

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2	THR
1	E	4	ASN
1	E	11	ARG
1	E	48	LEU
1	E	66	GLN
1	E	86	SER
1	E	156	VAL
1	E	237	LEU

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Mol	Chain	Res	Type
1	E	268	LYS
2	I	8	LYS
2	I	17	THR
2	I	26	THR
2	I	27	LEU
2	I	34	VAL
2	I	61	ASN
2	I	62	VAL

Sometimes 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	61	ASN
1	E	117	ASN
1	E	148	ASN
1	E	163	ASN
1	E	177	ASN
1	E	230	HIS
1	E	247	ASN
1	E	254	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.