



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 07:26 PM GMT

PDB ID : 2C7B
Title : THE CRYSTAL STRUCTURE OF ESTE1, A NEW THERMOPHILIC AND
THERMOSTABLE CARBOXYLESTERASE CLONED FROM A METAGENOMIC LIBRARY
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Deposited on : 2005-11-21
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

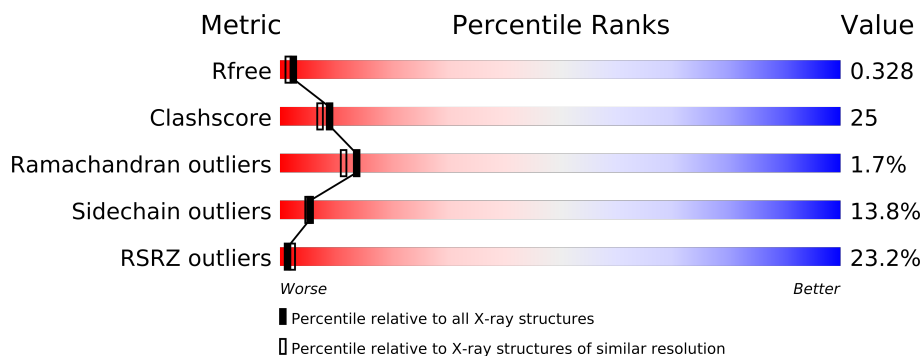
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


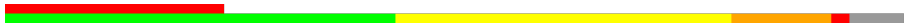
The reported resolution of this entry is 2.30 Å.

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	311	
1	B	311	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4607 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CARBOXYLESTERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	Se	12	0	1
			2248	1436	388	419	1	4			
1	B	291	Total	C	N	O	S	Se	0	0	1
			2221	1418	384	414	1	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	86	Total	O	0	0
			86	86		
2	B	52	Total	O	0	0
			52	52		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	73.71Å 73.71Å 234.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 28.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	76.1 (20.00-2.30) 98.5 (28.97-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.261 0.331 , 0.328	Depositor DCC
R_{free} test set	1513 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 10.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 38052 reflections	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	4607	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.59	1/2294 (0.0%)	0.95	3/3114 (0.1%)
1	B	0.99	14/2267 (0.6%)	1.48	27/3077 (0.9%)
All	All	0.82	15/4561 (0.3%)	1.25	30/6191 (0.5%)

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	B	0	1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	115	ALA	C-N	21.80	1.75	1.34
1	B	203	THR	C-N	-11.89	1.06	1.34
1	B	114	LEU	C-N	9.98	1.56	1.34
1	B	98	ARG	C-N	-9.69	1.11	1.34
1	B	120	PHE	C-N	7.26	1.48	1.34

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	PRO	CA-N-CD	-33.87	64.08	111.50
1	B	121	PRO	CA-N-CD	-32.45	66.07	111.50
1	A	120	PHE	C-N-CD	-23.48	68.93	120.60
1	B	203	THR	O-C-N	-14.45	99.57	122.70
1	A	120	PHE	C-N-CA	13.16	177.27	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	203	THR	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2248	0	2251	86	0
1	B	2221	0	2214	146	1
2	A	86	0	0	3	0
2	B	52	0	0	2	0
All	All	4607	0	4465	227	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

The worst 5 of 227 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:115:ALA:C	1:B:116:PRO:N	1.75	1.37
1:B:243:ALA:HB3	1:B:264:MSE:HE1	1.37	1.07
1:B:115:ALA:CA	1:B:116:PRO:N	2.20	1.03
1:B:264:MSE:HE2	1:B:271:ALA:HB2	1.39	1.02
1:A:265:LYS:HZ1	1:A:271:ALA:N	1.59	1.01

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	Distance(Å)	Clash(Å)
1:B:139:ASP:N	1:B:221:ARG:NH2[6_455]	1.63	0.57

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	A	293/311 (94%)	280 (96%)	9 (3%)	4 (1%)	16	15
1	B	289/311 (93%)	262 (91%)	21 (7%)	6 (2%)	11	8
All	All	582/622 (94%)	542 (93%)	30 (5%)	10 (2%)	14	11

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	PRO
1	A	222	PRO
1	B	40	ALA
1	B	41	VAL
1	B	46	ALA

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	A	233/244 (96%)	204 (88%)	29 (12%)	7	7
1	B	230/244 (94%)	195 (85%)	35 (15%)	4	4
All	All	463/488 (95%)	399 (86%)	64 (14%)	5	5

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	ARG
1	B	64	VAL
1	B	223	GLU
1	B	34	SER
1	B	45	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	33	GLN
1	A	309	GLN
1	B	186	ASN
1	B	309	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	295/311 (94%)	1.45	62 (21%) 1 3	6, 16, 32, 42	3 (1%)
1	B	291/311 (93%)	1.46	74 (25%) 1 2	0, 0, 0, 0	0
All	All	586/622 (94%)	1.45	136 (23%) 1 2	0, 7, 28, 42	3 (0%)

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	SER	9.9
1	B	41	VAL	6.8
1	B	121	PRO	5.6
1	B	310	PRO	5.6
1	B	33	GLN	5.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.