



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2026 – 04:22 AM UTC

PDB ID : 5IVH / pdb_00005ivh
Title : The alpha-esterase-7 carboxylesterase, E3, from the blowfly *Lucilia cuprina*:
apo-enzyme ensemble refinement
Authors : Correy, G.J.; Jackson, C.J.
Deposited on : 2016-03-20
Resolution : 1.71 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

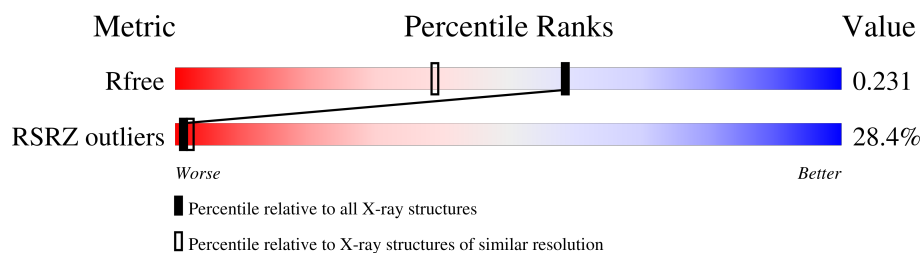
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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}	180053	1039 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 407711 atoms, of which 197120 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 Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	2-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	3-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	4-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	5-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	6-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	7-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	8-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	9-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	10-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	11-A	566	Total	C	H	N	O	S	0	0	

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	18-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	19-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	20-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	21-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	22-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	23-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	24-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	25-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	26-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	27-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	28-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	29-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	30-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	31-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	32-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	33-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	34-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	39-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	40-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	41-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	42-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	43-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	44-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q25252
A	-5	HIS	-	expression tag	UNP Q25252
A	-4	HIS	-	expression tag	UNP Q25252
A	-3	HIS	-	expression tag	UNP Q25252
A	-2	HIS	-	expression tag	UNP Q25252
A	-1	HIS	-	expression tag	UNP Q25252
A	0	HIS	-	expression tag	UNP Q25252
A	83	ALA	ASP	conflict	UNP Q25252
A	364	LEU	MET	conflict	UNP Q25252
A	419	PHE	ILE	conflict	UNP Q25252
A	472	THR	ALA	conflict	UNP Q25252
A	505	THR	ILE	conflict	UNP Q25252
A	530	GLU	LYS	conflict	UNP Q25252
A	554	GL			

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	4-A	222	Total 222	O 222	0	0
2	5-A	230	Total 230	O 230	0	0
2	6-A	233	Total 233	O 233	0	0
2	7-A	241	Total 241	O 241	0	0
2	8-A	238	Total 238	O 238	0	0
2	9-A	218	Total 218	O 218	0	0
2	10-A	217	Total 217	O 217	0	0
2	11-A	219	Total 219	O 219	0	0
2	12-A	231	Total 231	O 231	0	0
2	13-A	231	Total 231	O 231	0	0
2	14-A	235	Total 235	O 235	0	0
2	15-A	226	Total 226	O 226	0	0
2	16-A	230	Total 230	O 230	0	0
2	17-A	211	Total 211	O 211	0	0
2	18-A	228	Total 228	O 228	0	0
2	19-A	228	Total 228	O 228	0	0
2	20-A	236	Total 236	O 236	0	0
2	21-A	234	Total 234	O 234	0	0
2	22-A	225	Total 225	O 225	0	0
2	23-A	206	Total 206	O 206	0	0
2	24-A	218	Total 218	O 218	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	25-A	227	Total 227	O 227	0	0
2	26-A	227	Total 227	O 227	0	0
2	27-A	214	Total 214	O 214	0	0
2	28-A	237	Total 237	O 237	0	0
2	29-A	238	Total 238	O 238	0	0
2	30-A	237	Total 237	O 237	0	0
2	31-A	224	Total 224	O 224	0	0
2	32-A	224	Total 224	O 224	0	0
2	33-A	224	Total 224	O 224	0	0
2	34-A	235	Total 235	O 235	0	0
2	35-A	227	Total 227	O 227	0	0
2	36-A	236	Total 236	O 236	0	0
2	37-A	234	Total 234	O 234	0	0
2	38-A	244	Total 244	O 244	0	0
2	39-A	231	Total 231	O 231	0	0
2	40-A	231	Total 231	O 231	0	0
2	41-A	242	Total 242	O 242	0	0
2	42-A	246	Total 246	O 246	0	0
2	43-A	233	Total 233	O 233	0	0
2	44-A	223	Total 223	O 223	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	48.57Å 100.47Å 221.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.76 – 1.71 45.76 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.76-1.71) 91.5 (45.76-1.71)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 1.71Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.167 , 0.208 0.189 , 0.231	Depositor DCC
R_{free} test set	3002 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	407711	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	1-A	566/577 (98%)	1.72	161 (28%) ⓘ ⓘ	1, 1, 1, 1	566 (100%)
1	2-A	0/577	-	-	-	-
1	3-A	0/577	-	-	-	-
1	4-A	0/577	-	-	-	-
1	5-A	0/577	-	-	-	-
1	6-A	0/577	-	-	-	-
1	7-A	0/577	-	-	-	-
1	8-A	0/577	-	-	-	-
1	9-A	0/577	-	-	-	-
1	10-A	0/577	-	-	-	-
1	11-A	0/577	-	-	-	-
1	12-A	0/577	-	-	-	-
1	13-A	0/577	-	-	-	-
1	14-A	0/577	-	-	-	-
1	15-A	0/577	-	-	-	-
1	16-A	0/577	-	-	-	-
1	17-A	0/577	-	-	-	-
1	18-A	0/577	-	-	-	-
1	19-A	0/577	-	-	-	-
1	20-A	0/577	-	-	-	-
1	21-A	0/577	-	-	-	-
1	22-A	0/577	-	-	-	-
1	23-A	0/577	-	-	-	-
1	24-A	0/577	-	-	-	-
1	25-A	0/577	-	-	-	-
1	26-A	0/577	-	-	-	-
1	27-A	0/577	-	-	-	-
1	28-A	0/577	-	-	-	-
1	29-A	0/577	-	-	-	-
1	30-A	0/577	-	-	-	-
1	31-A					

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	33-A	0/577	-	-	-	-
1	34-A	0/577	-	-	-	-
1	35-A	0/577	-	-	-	-
1	36-A	0/577	-	-	-	-
1	37-A	0/577	-	-	-	-
1	38-A	0/577	-	-	-	-
1	39-A	0/577	-	-	-	-
1	40-A	0/577	-	-	-	-
1	41-A	0/577	-	-	-	-
1	42-A	0/577	-	-	-	-
1	43-A	0/577	-	-	-	-
1	44-A	0/577	-	-	-	-
All	All	566/25388 (2%)	1.72	161 (28%) 1 2	1, 1, 1, 1	566 (100%)

The worst 5 of 161 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	5	VAL	8.7
1	1-A	100	PHE	7.7
1	1-A	457	TYR	7.6
1	1-A	462	SER	7.6
1	1-A	463	GLY	7.5

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.