



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 04:24 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 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	:	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

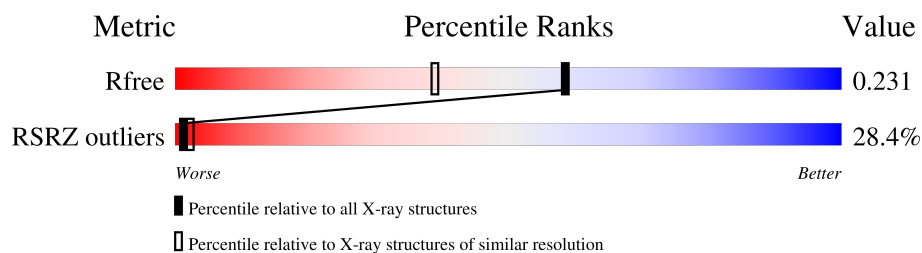
1 Overall quality at a glance

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	0
			9037	2911	4480	766	846	34			
1	12-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	13-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	14-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	15-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	16-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			

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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
1	35-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	36-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	37-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	GLY	ASP	conflict	UNP Q25252

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	234	Total	O	0	0
			234	234		
2	2-A	234	Total	O	0	0
			234	234		
2	3-A	224	Total	O	0	0
			224	224		

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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 O 227 227	0	0
2	26-A	227	Total O 227 227	0	0
2	27-A	214	Total O 214 214	0	0
2	28-A	237	Total O 237 237	0	0
2	29-A	238	Total O 238 238	0	0
2	30-A	237	Total O 237 237	0	0
2	31-A	224	Total O 224 224	0	0
2	32-A	224	Total O 224 224	0	0
2	33-A	224	Total O 224 224	0	0
2	34-A	235	Total O 235 235	0	0
2	35-A	227	Total O 227 227	0	0
2	36-A	236	Total O 236 236	0	0
2	37-A	234	Total O 234 234	0	0
2	38-A	244	Total O 244 244	0	0
2	39-A	231	Total O 231 231	0	0
2	40-A	231	Total O 231 231	0	0
2	41-A	242	Total O 242 242	0	0
2	42-A	246	Total O 246 246	0	0
2	43-A	233	Total O 233 233	0	0
2	44-A	223	Total O 223 223	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](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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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	0/577	-	-	-	-
1	32-A	0/577	-	-	-	-

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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%)

All (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
1	1-A	101	ILE	7.3
1	1-A	362	MET	6.5
1	1-A	335	THR	6.3
1	1-A	22	PHE	5.6
1	1-A	8	MET	5.5
1	1-A	465	GLY	5.3
1	1-A	460	MET	5.2
1	1-A	78	ARG	5.2
1	1-A	354	PHE	5.2
1	1-A	436	THR	5.2
1	1-A	403	THR	5.1
1	1-A	359	LEU	5.0
1	1-A	438	GLY	5.0
1	1-A	102	THR	4.9
1	1-A	15	ILE	4.8
1	1-A	300	LEU	4.7
1	1-A	322	ASP	4.5
1	1-A	459	ILE	4.5
1	1-A	464	ARG	4.5
1	1-A	494	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	1-A	358	ILE	4.4
1	1-A	489	LYS	4.3
1	1-A	7	LEU	4.3
1	1-A	324	VAL	4.2
1	1-A	19	GLU	4.1
1	1-A	524	VAL	4.1
1	1-A	467	LYS	4.0
1	1-A	80	THR	4.0
1	1-A	193	MET	4.0
1	1-A	409	ALA	4.0
1	1-A	544	GLU	3.8
1	1-A	6	SER	3.8
1	1-A	386	THR	3.8
1	1-A	320	THR	3.8
1	1-A	434	ASN	3.6
1	1-A	466	VAL	3.6
1	1-A	439	THR	3.5
1	1-A	298	LEU	3.4
1	1-A	82	TRP	3.4
1	1-A	357	SER	3.4
1	1-A	125	THR	3.4
1	1-A	122	ASN	3.4
1	1-A	437	SER	3.4
1	1-A	321	ALA	3.3
1	1-A	435	HIS	3.3
1	1-A	406	THR	3.3
1	1-A	93	ASP	3.3
1	1-A	329	PRO	3.3
1	1-A	364	LEU	3.3
1	1-A	176	ASN	3.3
1	1-A	328	HIS	3.2
1	1-A	308	MET	3.2
1	1-A	232	GLN	3.2
1	1-A	402	VAL	3.2
1	1-A	518	ILE	3.2
1	1-A	179	ASP	3.2
1	1-A	9	GLU	3.2
1	1-A	319	GLN	3.1
1	1-A	304	THR	3.1
1	1-A	234	ARG	3.1
1	1-A	27	LEU	3.1
1	1-A	286	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	1-A	177	SER	3.1
1	1-A	355	PHE	3.0
1	1-A	124	GLU	3.0
1	1-A	365	LEU	2.9
1	1-A	33	VAL	2.9
1	1-A	126	LYS	2.9
1	1-A	181	ASN	2.9
1	1-A	68	VAL	2.9
1	1-A	519	GLU	2.9
1	1-A	532	SER	2.9
1	1-A	451	GLU	2.8
1	1-A	273	ASP	2.8
1	1-A	565	LYS	2.8
1	1-A	545	LEU	2.8
1	1-A	361	GLN	2.8
1	1-A	301	GLU	2.8
1	1-A	332	MET	2.8
1	1-A	81	PRO	2.8
1	1-A	397	ILE	2.8
1	1-A	517	GLU	2.8
1	1-A	12	LYS	2.8
1	1-A	531	LYS	2.8
1	1-A	373	VAL	2.8
1	1-A	230	THR	2.8
1	1-A	280	GLU	2.7
1	1-A	392	GLU	2.7
1	1-A	388	PRO	2.6
1	1-A	570	PHE	2.6
1	1-A	525	SER	2.6
1	1-A	36	GLU	2.6
1	1-A	534	GLU	2.6
1	1-A	77	GLN	2.6
1	1-A	558	GLN	2.6
1	1-A	516	ASN	2.6
1	1-A	404	GLY	2.6
1	1-A	297	VAL	2.6
1	1-A	85	VAL	2.5
1	1-A	231	GLU	2.5
1	1-A	103	GLY	2.5
1	1-A	14	LYS	2.5
1	1-A	523	ASN	2.5
1	1-A	258	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	246	ASN	2.5
1	1-A	267	ALA	2.5
1	1-A	18	ILE	2.5
1	1-A	104	LYS	2.5
1	1-A	405	GLU	2.5
1	1-A	284	LYS	2.4
1	1-A	87	ASP	2.4
1	1-A	105	VAL	2.4
1	1-A	530	GLU	2.4
1	1-A	433	PHE	2.4
1	1-A	368	GLU	2.3
1	1-A	13	TRP	2.3
1	1-A	39	TYR	2.3
1	1-A	442	TYR	2.3
1	1-A	333	VAL	2.3
1	1-A	121	LEU	2.3
1	1-A	295	GLU	2.3
1	1-A	389	GLU	2.3
1	1-A	410	ASP	2.3
1	1-A	400	ALA	2.3
1	1-A	341	ILE	2.3
1	1-A	363	PRO	2.2
1	1-A	180	LEU	2.2
1	1-A	236	LEU	2.2
1	1-A	292	LYS	2.2
1	1-A	334	LYS	2.2
1	1-A	147	MET	2.2
1	1-A	248	ILE	2.2
1	1-A	541	ILE	2.2
1	1-A	384	GLU	2.2
1	1-A	99	ASP	2.2
1	1-A	422	TRP	2.2
1	1-A	370	GLU	2.2
1	1-A	412	PHE	2.2
1	1-A	367	LYS	2.2
1	1-A	535	VAL	2.1
1	1-A	106	CYS	2.1
1	1-A	235	GLY	2.1
1	1-A	245	GLY	2.1
1	1-A	526	TRP	2.1
1	1-A	527	ASP	2.1
1	1-A	477	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-A	204	ASN	2.1
1	1-A	90	ASN	2.1
1	1-A	288	GLN	2.1
1	1-A	515	SER	2.1
1	1-A	419	PHE	2.1
1	1-A	201	ASN	2.0
1	1-A	16	LYS	2.0
1	1-A	559	TRP	2.0
1	1-A	138	PHE	2.0
1	1-A	444	TYR	2.0

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.