



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 09:35 PM UTC

PDB ID : 5IVK / pdb_00005ivk
Title : The alpha-esterase-7 carboxylesterase, E3, from the blowfly *Lucilia cuprina*: phosphorylated-enzyme ensemble refinement
Authors : Correy, G.J.; Jackson, C.J.
Deposited on : 2016-03-21
Resolution : 1.53 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

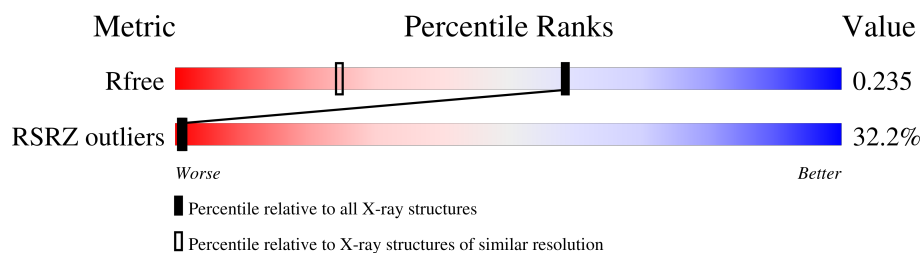
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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	1003 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 405539 atoms, of which 192984 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
			9035	2911	4478	766	846	34			
1	2-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	3-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	4-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	5-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	6-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	7-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	8-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	9-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	10-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	11-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	12-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	13-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	14-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	15-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	16-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	18-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	19-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	20-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	21-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	22-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	23-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	24-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	25-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	26-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	27-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	28-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	29-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	30-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	31-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	32-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	33-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	34-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	35-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	36-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0
1	37-A	566	Total 9035	C 2911	H 4478	N 766	O 846	S 34	0	0	0

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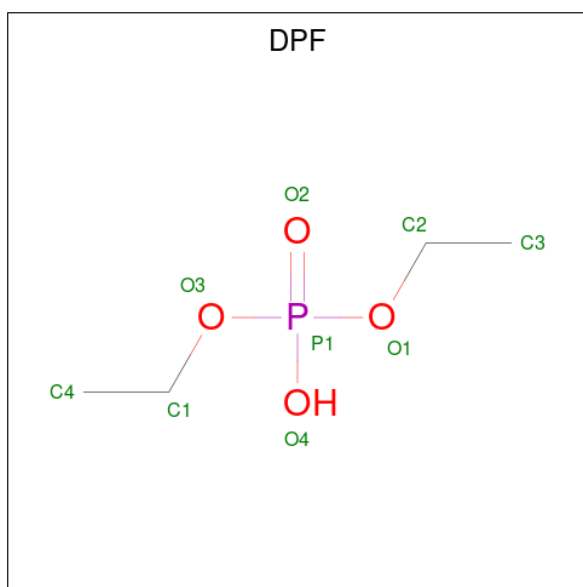
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	39-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	40-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	41-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	42-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	43-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			

There are 13 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	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 DIETHYL HYDROGEN PHOSPHATE (CCD ID: DPF) (formula: C₄H₁₁O₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	2-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	3-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	4-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	5-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	6-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	7-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	8-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	9-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	10-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	11-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	12-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	13-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	14-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	15-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	16-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	17-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	18-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	19-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	20-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	21-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	22-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	23-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	24-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	25-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	26-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	27-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	28-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	29-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	30-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	31-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	32-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	33-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	34-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	35-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	36-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	37-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	38-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	39-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	40-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	41-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	42-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	43-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	399	Total	O	0	0
			399	399		
3	2-A	380	Total	O	0	0
			380	380		
3	3-A	356	Total	O	0	0
			356	356		
3	4-A	389	Total	O	0	0
			389	389		
3	5-A	386	Total	O	0	0
			386	386		
3	6-A	379	Total	O	0	0
			379	379		
3	7-A	375	Total	O	0	0
			375	375		
3	8-A	365	Total	O	0	0
			365	365		
3	9-A	373	Total	O	0	0
			373	373		
3	10-A	365	Total	O	0	0
			365	365		
3	11-A	360	Total	O	0	0
			360	360		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	12-A	396	Total 396	O 396	0	0
3	13-A	406	Total 406	O 406	0	0
3	14-A	378	Total 378	O 378	0	0
3	15-A	374	Total 374	O 374	0	0
3	16-A	386	Total 386	O 386	0	0
3	17-A	357	Total 357	O 357	0	0
3	18-A	353	Total 353	O 353	0	0
3	19-A	363	Total 363	O 363	0	0
3	20-A	399	Total 399	O 399	0	0
3	21-A	389	Total 389	O 389	0	0
3	22-A	380	Total 380	O 380	0	0
3	23-A	376	Total 376	O 376	0	0
3	24-A	381	Total 381	O 381	0	0
3	25-A	359	Total 359	O 359	0	0
3	26-A	362	Total 362	O 362	0	0
3	27-A	379	Total 379	O 379	0	0
3	28-A	389	Total 389	O 389	0	0
3	29-A	377	Total 377	O 377	0	0
3	30-A	363	Total 363	O 363	0	0
3	31-A	365	Total 365	O 365	0	0
3	32-A	393	Total 393	O 393	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	33-A	378	Total 378	O 378	0	0
3	34-A	384	Total 384	O 384	0	0
3	35-A	383	Total 383	O 383	0	0
3	36-A	390	Total 390	O 390	0	0
3	37-A	358	Total 358	O 358	0	0
3	38-A	377	Total 377	O 377	0	0
3	39-A	393	Total 393	O 393	0	0
3	40-A	388	Total 388	O 388	0	0
3	41-A	390	Total 390	O 390	0	0
3	42-A	390	Total 390	O 390	0	0
3	43-A	377	Total 377	O 377	0	0

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

3 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	51.82Å 101.25Å 225.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.01 – 1.53 42.01 – 1.53	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.01-1.53) 95.8 (42.01-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.53Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.181 , 0.220 0.193 , 0.235	Depositor DCC
R_{free} test set	4499 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	405539	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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](#)

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

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](#)

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](#)

43 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DPF	34-A	601	1	4,7,8	0.93	0	2,7,10	0.44	0
2	DPF	8-A	601	1	4,7,8	0.94	0	2,7,10	0.37	0
2	DPF	23-A	601	1	4,7,8	0.92	0	2,7,10	0.38	0
2	DPF	28-A	601	1	4,7,8	0.90	0	2,7,10	0.09	0
2	DPF	30-A	601	1	4,7,8	1.06	0	2,7,10	0.58	0
2	DPF	17-A	601	1	4,7,8	0.98	0	2,7,10	0.06	0
2	DPF	40-A	601	1	4,7,8	1.00	0	2,7,10	0.28	0
2	DPF	3-A	601	1	4,7,8	1.04	0	2,7,10	0.30	0
2	DPF	1-A	601	1	4,7,8	1.24	1 (25%)	2,7,10	0.42	0
2	DPF	38-A	601	1	4,7,8	0.93	0	2,7,10	0.68	0
2	DPF	39-A	601	1	4,7,8	0.89	0	2,7,10	0.34	0
2	DPF	10-A	601	1	4,7,8	0.87	0	2,7,10	0.70	0
2	DPF	13-A	601	1	4,7,8	1.15	0	2,7,10	0.43	0
2	DPF	41-A	601	1	4,7,8	0.79	0	2,7,10	0.26	0
2	DPF	21-A	601	1	4,7,8	0.99	0	2,7,10	0.13	0
2	DPF	11-A	601	1	4,7,8	1.09	0	2,7,10	0.64	0
2	DPF	32-A	601	1	4,7,8	0.56	0	2,7,10	0.38	0
2	DPF	14-A	601	1	4,7,8	0.97	0	2,7,10	0.23	0
2	DPF	19-A	601	1	4,7,8	0.89	0	2,7,10	0.79	0
2	DPF	27-A	601	1	4,7,8	0.99	0	2,7,10	0.59	0
2	DPF	42-A	601	1	4,7,8	0.78	0	2,7,10	0.38	0
2	DPF	31-A	601	1	4,7,8	0.74	0	2,7,10	0.09	0
2	DPF	29-A	601	1	4,7,8	0.98	0	2,7,10	0.52	0
2	DPF	9-A	601	1	4,7,8	1.10	0	2,7,10	0.35	0
2	DPF	2-A	601	1	4,7,8	1.12	0	2,7,10	0.72	0
2	DPF	4-A	601	1	4,7,8	0.86	0	2,7,10	1.12	0
2	DPF	18-A	601	1	4,7,8	1.00	0	2,7,10	0.90	0
2	DPF	16-A	601	1	4,7,8	0.98	0	2,7,10	0.64	0
2	DPF	7-A	601	1	4,7,8	1.00	0	2,7,10	0.53	0
2	DPF	15-A	601	1	4,7,8	1.44	1 (25%)	2,7,10	0.97	0
2	DPF	33-A	601	1	4,7,8	1.08	0	2,7,10	1.09	0
2	DPF	35-A	601	1	4,7,8	1.03	0	2,7,10	0.57	0
2	DPF	36-A	601	1	4,7,8	0.82	0	2,7,10	0.19	0
2	DPF	6-A	601	1	4,7,8	1.10	0	2,7,10	0.97	0
2	DPF	12-A	601	1	4,7,8	1.01	0	2,7,10	0.74	0
2	DPF	37-A	601	1	4,7,8	0.88	0	2,7,10	0.68	0
2	DPF	5-A	601	1	4,7,8	0.79	0	2,7,10	0.19	0
2	DPF	24-A	601	1	4,7,8	0.97	0	2,7,10	0.39	0
2	DPF	22-A	601	1	4,7,8	1.19	1 (25%)	2,7,10	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DPF	20-A	601	1	4,7,8	1.02	0	2,7,10	0.30	0
2	DPF	43-A	601	1	4,7,8	0.98	0	2,7,10	0.60	0
2	DPF	25-A	601	1	4,7,8	0.91	0	2,7,10	0.66	0
2	DPF	26-A	601	1	4,7,8	0.74	0	2,7,10	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DPF	34-A	601	1	-	1/2/6/8	-
2	DPF	8-A	601	1	-	0/2/6/8	-
2	DPF	23-A	601	1	-	0/2/6/8	-
2	DPF	28-A	601	1	-	1/2/6/8	-
2	DPF	30-A	601	1	-	1/2/6/8	-
2	DPF	17-A	601	1	-	0/2/6/8	-
2	DPF	40-A	601	1	-	0/2/6/8	-
2	DPF	3-A	601	1	-	0/2/6/8	-
2	DPF	1-A	601	1	-	2/2/6/8	-
2	DPF	38-A	601	1	-	0/2/6/8	-
2	DPF	39-A	601	1	-	1/2/6/8	-
2	DPF	10-A	601	1	-	0/2/6/8	-
2	DPF	13-A	601	1	-	2/2/6/8	-
2	DPF	41-A	601	1	-	0/2/6/8	-
2	DPF	21-A	601	1	-	0/2/6/8	-
2	DPF	11-A	601	1	-	2/2/6/8	-
2	DPF	32-A	601	1	-	0/2/6/8	-
2	DPF	14-A	601	1	-	1/2/6/8	-
2	DPF	19-A	601	1	-	0/2/6/8	-
2	DPF	27-A	601	1	-	0/2/6/8	-
2	DPF	42-A	601	1	-	0/2/6/8	-
2	DPF	31-A	601	1	-	0/2/6/8	-
2	DPF	29-A	601	1	-	0/2/6/8	-
2	DPF	9-A	601	1	-	1/2/6/8	-
2	DPF	2-A	601	1	-	0/2/6/8	-
2	DPF	4-A	601	1	-	0/2/6/8	-
2	DPF	18-A	601	1	-	0/2/6/8	-
2	DPF	16-A	601	1	-	0/2/6/8	-
2	DPF	7-A	601	1	-	0/2/6/8	-
2	DPF	15-A	601	1	-	1/2/6/8	-
2	DPF	33-A	601	1	-	1/2/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DPF	35-A	601	1	-	0/2/6/8	-
2	DPF	36-A	601	1	-	0/2/6/8	-
2	DPF	6-A	601	1	-	1/2/6/8	-
2	DPF	12-A	601	1	-	1/2/6/8	-
2	DPF	37-A	601	1	-	0/2/6/8	-
2	DPF	5-A	601	1	-	0/2/6/8	-
2	DPF	24-A	601	1	-	0/2/6/8	-
2	DPF	22-A	601	1	-	1/2/6/8	-
2	DPF	20-A	601	1	-	0/2/6/8	-
2	DPF	43-A	601	1	-	0/2/6/8	-
2	DPF	25-A	601	1	-	1/2/6/8	-
2	DPF	26-A	601	1	-	1/2/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	15-A	601	DPF	O1-C2	-2.23	1.37	1.44
2	1-A	601	DPF	O1-C2	-2.05	1.38	1.44
2	22-A	601	DPF	O1-C2	-2.02	1.38	1.44

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1-A	601	DPF	C4-C1-O3-P1
2	1-A	601	DPF	C3-C2-O1-P1
2	6-A	601	DPF	C4-C1-O3-P1
2	9-A	601	DPF	C4-C1-O3-P1
2	11-A	601	DPF	C4-C1-O3-P1
2	11-A	601	DPF	C3-C2-O1-P1
2	12-A	601	DPF	C3-C2-O1-P1
2	13-A	601	DPF	C4-C1-O3-P1
2	13-A	601	DPF	C3-C2-O1-P1
2	14-A	601	DPF	C4-C1-O3-P1
2	15-A	601	DPF	C4-C1-O3-P1
2	22-A	601	DPF	C3-C2-O1-P1
2	25-A	601	DPF	C4-C1-O3-P1
2	26-A	601	DPF	C4-C1-O3-P1
2	28-A	601	DPF	C4-C1-O3-P1
2	30-A	601	DPF	C4-C1-O3-P1

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Mol	Chain	Res	Type	Atoms
2	33-A	601	DPF	C4-C1-O3-P1
2	34-A	601	DPF	C4-C1-O3-P1
2	39-A	601	DPF	C4-C1-O3-P1

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	32-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
32	A	125:THR	C	126:LYS	N	1.82

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%)	1.70	182 (32%) ⓘ ⓘ	0, 0, 0, 0	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	-	-	-	-
All	All	566/24811 (2%)	1.70	182 (32%) 1 1	0, 0, 0, 0	566 (100%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	515	SER	8.2
1	1-A	514	TYR	7.9
1	1-A	100	PHE	7.7
1	1-A	519	GLU	7.2
1	1-A	518	ILE	6.8
1	1-A	520	GLY	6.8
1	1-A	521	MET	6.6
1	1-A	381	ALA	6.4
1	1-A	383	ALA	6.4
1	1-A	517	GLU	6.1
1	1-A	522	GLU	5.9
1	1-A	124	GLU	5.8
1	1-A	384	GLU	5.7
1	1-A	361	GLN	5.7
1	1-A	362	MET	4.9
1	1-A	532	SER	4.9
1	1-A	451	GLU	4.8
1	1-A	319	GLN	4.7
1	1-A	513	PRO	4.7
1	1-A	104	LYS	4.5
1	1-A	179	ASP	4.5
1	1-A	102	THR	4.4
1	1-A	382	ASP	4.4
1	1-A	90	ASN	4.2
1	1-A	295	GLU	4.2
1	1-A	392	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	122	ASN	4.1
1	1-A	36	GLU	4.1
1	1-A	101	ILE	4.1
1	1-A	25	TYR	4.1
1	1-A	360	LYS	4.0
1	1-A	516	ASN	4.0
1	1-A	125	THR	4.0
1	1-A	92	LYS	3.9
1	1-A	301	GLU	3.9
1	1-A	77	GLN	3.8
1	1-A	460	MET	3.7
1	1-A	527	ASP	3.7
1	1-A	537	LYS	3.7
1	1-A	355	PHE	3.7
1	1-A	466	VAL	3.6
1	1-A	396	LYS	3.6
1	1-A	23	LEU	3.6
1	1-A	280	GLU	3.5
1	1-A	461	ARG	3.5
1	1-A	31	GLU	3.4
1	1-A	12	LYS	3.4
1	1-A	486	ARG	3.4
1	1-A	248	ILE	3.4
1	1-A	22	PHE	3.4
1	1-A	386	THR	3.3
1	1-A	523	ASN	3.2
1	1-A	433	PHE	3.2
1	1-A	549	ASP	3.2
1	1-A	431	LEU	3.2
1	1-A	322	ASP	3.2
1	1-A	505	THR	3.2
1	1-A	284	LYS	3.2
1	1-A	564	GLU	3.2
1	1-A	105	VAL	3.2
1	1-A	87	ASP	3.1
1	1-A	450	SER	3.1
1	1-A	465	GLY	3.1
1	1-A	289	ASP	3.1
1	1-A	334	LYS	3.1
1	1-A	236	LEU	3.1
1	1-A	365	LEU	3.1
1	1-A	405	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	1-A	441	VAL	3.1
1	1-A	359	LEU	3.1
1	1-A	389	GLU	3.1
1	1-A	534	GLU	3.1
1	1-A	364	LEU	3.0
1	1-A	13	TRP	3.0
1	1-A	91	HIS	3.0
1	1-A	103	GLY	3.0
1	1-A	489	LYS	3.0
1	1-A	544	GLU	2.9
1	1-A	24	ASN	2.9
1	1-A	5	VAL	2.9
1	1-A	7	LEU	2.9
1	1-A	531	LYS	2.9
1	1-A	490	GLU	2.9
1	1-A	200	ASN	2.9
1	1-A	510	THR	2.9
1	1-A	292	LYS	2.9
1	1-A	470	SER	2.9
1	1-A	434	ASN	2.8
1	1-A	80	THR	2.8
1	1-A	357	SER	2.8
1	1-A	452	ASP	2.8
1	1-A	303	ARG	2.8
1	1-A	78	ARG	2.7
1	1-A	14	LYS	2.7
1	1-A	52	ASP	2.7
1	1-A	459	ILE	2.7
1	1-A	16	LYS	2.7
1	1-A	253	ASN	2.7
1	1-A	261	PHE	2.7
1	1-A	420	TYR	2.6
1	1-A	290	LEU	2.6
1	1-A	18	ILE	2.6
1	1-A	530	GLU	2.6
1	1-A	157	ASP	2.6
1	1-A	294	GLU	2.6
1	1-A	368	GLU	2.6
1	1-A	437	SER	2.6
1	1-A	435	HIS	2.6
1	1-A	358	ILE	2.5
1	1-A	85	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	123	PRO	2.5
1	1-A	363	PRO	2.5
1	1-A	126	LYS	2.5
1	1-A	464	ARG	2.5
1	1-A	278	VAL	2.5
1	1-A	8	MET	2.5
1	1-A	529	ILE	2.5
1	1-A	276	LYS	2.5
1	1-A	375	PHE	2.5
1	1-A	68	VAL	2.5
1	1-A	70	GLU	2.4
1	1-A	34	VAL	2.4
1	1-A	204	ASN	2.4
1	1-A	412	PHE	2.4
1	1-A	175	LEU	2.4
1	1-A	403	THR	2.4
1	1-A	565	LYS	2.4
1	1-A	273	ASP	2.3
1	1-A	568	ASP	2.3
1	1-A	387	ALA	2.3
1	1-A	526	TRP	2.3
1	1-A	406	THR	2.3
1	1-A	269	TYR	2.3
1	1-A	367	LYS	2.3
1	1-A	345	MET	2.3
1	1-A	215	PHE	2.3
1	1-A	354	PHE	2.3
1	1-A	93	ASP	2.3
1	1-A	457	TYR	2.3
1	1-A	89	CYS	2.2
1	1-A	146	ASP	2.2
1	1-A	570	PHE	2.2
1	1-A	366	VAL	2.2
1	1-A	494	TYR	2.2
1	1-A	267	ALA	2.2
1	1-A	17	CYS	2.2
1	1-A	304	THR	2.2
1	1-A	281	PHE	2.2
1	1-A	65	GLN	2.2
1	1-A	543	ASP	2.2
1	1-A	180	LEU	2.2
1	1-A	266	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	369	LEU	2.2
1	1-A	286	LYS	2.2
1	1-A	296	LYS	2.2
1	1-A	528	PRO	2.2
1	1-A	469	VAL	2.2
1	1-A	141	GLY	2.1
1	1-A	463	GLY	2.1
1	1-A	480	TRP	2.1
1	1-A	20	ASN	2.1
1	1-A	394	GLY	2.1
1	1-A	542	SER	2.1
1	1-A	27	LEU	2.1
1	1-A	19	GLU	2.1
1	1-A	331	GLU	2.1
1	1-A	533	ASP	2.1
1	1-A	393	MET	2.1
1	1-A	98	VAL	2.1
1	1-A	535	VAL	2.1
1	1-A	28	THR	2.1
1	1-A	112	LEU	2.1
1	1-A	512	ASN	2.1
1	1-A	419	PHE	2.0
1	1-A	507	PHE	2.0
1	1-A	182	VAL	2.0
1	1-A	524	VAL	2.0
1	1-A	86	ARG	2.0
1	1-A	305	ASN	2.0
1	1-A	335	THR	2.0
1	1-A	388	PRO	2.0
1	1-A	152	TYR	2.0

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

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

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DPF	1-A	601	8/9	0.92	0.13	16,16,16,16	18
2	DPF	2-A	601	8/9	-	-	16,16,17,17	18
2	DPF	3-A	601	8/9	-	-	16,16,16,16	18
2	DPF	4-A	601	8/9	-	-	16,16,16,16	18
2	DPF	5-A	601	8/9	-	-	16,16,16,17	18
2	DPF	6-A	601	8/9	-	-	16,16,16,17	18
2	DPF	7-A	601	8/9	-	-	16,16,16,17	18
2	DPF	8-A	601	8/9	-	-	16,16,17,17	18
2	DPF	9-A	601	8/9	-	-	16,16,16,16	18
2	DPF	10-A	601	8/9	-	-	16,16,16,17	18
2	DPF	11-A	601	8/9	-	-	16,16,16,17	18
2	DPF	12-A	601	8/9	-	-	16,16,16,16	18
2	DPF	13-A	601	8/9	-	-	16,16,16,16	18
2	DPF	14-A	601	8/9	-	-	16,16,16,17	18
2	DPF	15-A	601	8/9	-	-	16,16,17,17	18
2	DPF	16-A	601	8/9	-	-	16,16,16,16	18
2	DPF	17-A	601	8/9	-	-	16,16,16,16	18
2	DPF	18-A	601	8/9	-	-	16,16,17,17	18
2	DPF	19-A	601	8/9	-	-	16,16,16,16	18
2	DPF	20-A	601	8/9	-	-	16,16,16,16	18
2	DPF	21-A	601	8/9	-	-	16,16,16,16	18
2	DPF	22-A	601	8/9	-	-	16,16,16,16	18
2	DPF	23-A	601	8/9	-	-	16,16,16,16	18
2	DPF	24-A	601	8/9	-	-	16,16,16,16	18
2	DPF	25-A	601	8/9	-	-	16,16,17,17	18
2	DPF	26-A	601	8/9	-	-	16,16,17,17	18
2	DPF	27-A	601	8/9	-	-	16,16,16,16	18
2	DPF	28-A	601	8/9	-	-	16,16,16,16	18
2	DPF	29-A	601	8/9	-	-	16,16,16,16	18
2	DPF	30-A	601	8/9	-	-	16,16,17,17	18
2	DPF	31-A	601	8/9	-	-	16,16,17,17	18
2	DPF	32-A	601	8/9	-	-	16,16,17,17	18
2	DPF	33-A	601	8/9	-	-	16,16,17,17	18
2	DPF	34-A	601	8/9	-	-	16,16,17,17	18
2	DPF	35-A	601	8/9	-	-	16,16,17,17	18
2	DPF	36-A	601	8/9	-	-	16,16,17,17	18
2	DPF	37-A	601	8/9	-	-	16,16,16,16	18

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DPF	38-A	601	8/9	-	-	16,16,17,17	18
2	DPF	39-A	601	8/9	-	-	16,16,16,16	18
2	DPF	40-A	601	8/9	-	-	16,16,16,17	18
2	DPF	41-A	601	8/9	-	-	16,16,17,17	18
2	DPF	42-A	601	8/9	-	-	16,16,16,17	18
2	DPF	43-A	601	8/9	-	-	16,16,16,17	18

5.5 Other polymers [i](#)

There are no such residues in this entry.