



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2016 – 05:19 AM EDT

PDB ID : 5HFN
Title : Crystal structure of a loop truncation variant of *Thermotoga maritima* Acetyl Esterase TM0077 (apo structure) at 2.75 Angstrom resolution
Authors : Manoj, N.; Singh, M.K.
Deposited on : 2016-01-07
Resolution : 2.75 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

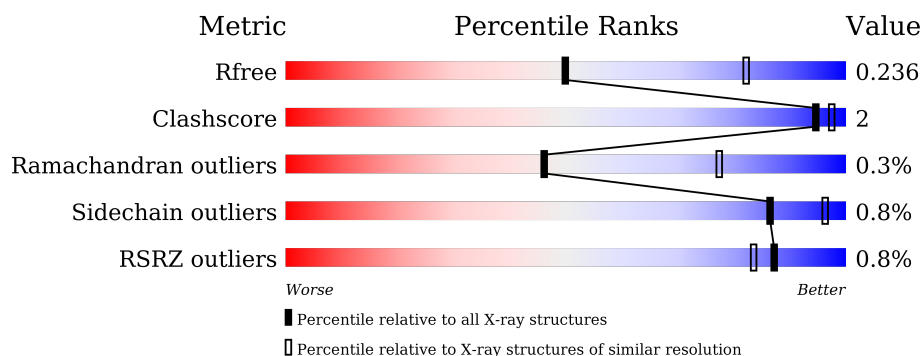
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	311	<div> <div>85%</div> <div>5%</div> <div>10%</div> </div>
1	B	311	<div> <div>83%</div> <div>6%</div> <div>11%</div> </div>
1	C	311	<div> <div>2%</div> <div>84%</div> <div>6%</div> <div>10%</div> </div>
1	D	311	<div> <div>%</div> <div>86%</div> <div>5%</div> <div>9%</div> </div>
1	E	311	<div> <div>%</div> <div>83%</div> <div>6%</div> <div>10%</div> </div>
1	F	311	<div> <div>83%</div> <div>7%</div> <div>10%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13326 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 Cephalosporin-C deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2187	1425	363	390	9			
1	B	278	Total	C	N	O	S	0	1	0
			2196	1436	361	390	9			
1	C	279	Total	C	N	O	S	0	1	0
			2195	1436	360	390	9			
1	D	283	Total	C	N	O	S	0	1	0
			2201	1444	356	391	10			
1	E	279	Total	C	N	O	S	0	1	0
			2222	1450	365	398	9			
1	F	279	Total	C	N	O	S	0	1	0
			2240	1461	370	400	9			

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9WXT2
A	-10	GLY	-	expression tag	UNP Q9WXT2
A	-9	SER	-	expression tag	UNP Q9WXT2
A	-8	ASP	-	expression tag	UNP Q9WXT2
A	-7	LYS	-	expression tag	UNP Q9WXT2
A	-6	ILE	-	expression tag	UNP Q9WXT2
A	-5	HIS	-	expression tag	UNP Q9WXT2
A	-4	HIS	-	expression tag	UNP Q9WXT2
A	-3	HIS	-	expression tag	UNP Q9WXT2
A	-2	HIS	-	expression tag	UNP Q9WXT2
A	-1	HIS	-	expression tag	UNP Q9WXT2
A	0	HIS	-	expression tag	UNP Q9WXT2
A	?	-	GLN	deletion	UNP Q9WXT2
A	?	-	GLY	deletion	UNP Q9WXT2
A	?	-	SER	deletion	UNP Q9WXT2
A	?	-	GLY	deletion	UNP Q9WXT2
A	?	-	TRP	deletion	UNP Q9WXT2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP Q9WXT2
A	?	-	LYS	deletion	UNP Q9WXT2
A	?	-	GLY	deletion	UNP Q9WXT2
A	?	-	ASP	deletion	UNP Q9WXT2
A	?	-	THR	deletion	UNP Q9WXT2
A	?	-	PRO	deletion	UNP Q9WXT2
A	?	-	ASP	deletion	UNP Q9WXT2
A	?	-	TYR	deletion	UNP Q9WXT2
A	?	-	PRO	deletion	UNP Q9WXT2
A	?	-	GLU	deletion	UNP Q9WXT2
A	?	-	GLY	deletion	UNP Q9WXT2
A	?	-	PRO	deletion	UNP Q9WXT2
A	?	-	VAL	deletion	UNP Q9WXT2
A	?	-	ASP	deletion	UNP Q9WXT2
A	?	-	PRO	deletion	UNP Q9WXT2
A	?	-	GLN	deletion	UNP Q9WXT2
A	?	-	TYR	deletion	UNP Q9WXT2
A	?	-	PRO	deletion	UNP Q9WXT2
A	?	-	GLY	deletion	UNP Q9WXT2
A	?	-	PHE	deletion	UNP Q9WXT2
A	?	-	MET	deletion	UNP Q9WXT2
B	-11	MET	-	initiating methionine	UNP Q9WXT2
B	-10	GLY	-	expression tag	UNP Q9WXT2
B	-9	SER	-	expression tag	UNP Q9WXT2
B	-8	ASP	-	expression tag	UNP Q9WXT2
B	-7	LYS	-	expression tag	UNP Q9WXT2
B	-6	ILE	-	expression tag	UNP Q9WXT2
B	-5	HIS	-	expression tag	UNP Q9WXT2
B	-4	HIS	-	expression tag	UNP Q9WXT2
B	-3	HIS	-	expression tag	UNP Q9WXT2
B	-2	HIS	-	expression tag	UNP Q9WXT2
B	-1	HIS	-	expression tag	UNP Q9WXT2
B	0	HIS	-	expression tag	UNP Q9WXT2
B	?	-	GLN	deletion	UNP Q9WXT2
B	?	-	GLY	deletion	UNP Q9WXT2
B	?	-	SER	deletion	UNP Q9WXT2
B	?	-	GLY	deletion	UNP Q9WXT2
B	?	-	TRP	deletion	UNP Q9WXT2
B	?	-	LEU	deletion	UNP Q9WXT2
B	?	-	LYS	deletion	UNP Q9WXT2
B	?	-	GLY	deletion	UNP Q9WXT2
B	?	-	ASP	deletion	UNP Q9WXT2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP Q9WXT2
B	?	-	PRO	deletion	UNP Q9WXT2
B	?	-	ASP	deletion	UNP Q9WXT2
B	?	-	TYR	deletion	UNP Q9WXT2
B	?	-	PRO	deletion	UNP Q9WXT2
B	?	-	GLU	deletion	UNP Q9WXT2
B	?	-	GLY	deletion	UNP Q9WXT2
B	?	-	PRO	deletion	UNP Q9WXT2
B	?	-	VAL	deletion	UNP Q9WXT2
B	?	-	ASP	deletion	UNP Q9WXT2
B	?	-	PRO	deletion	UNP Q9WXT2
B	?	-	GLN	deletion	UNP Q9WXT2
B	?	-	TYR	deletion	UNP Q9WXT2
B	?	-	PRO	deletion	UNP Q9WXT2
B	?	-	GLY	deletion	UNP Q9WXT2
B	?	-	PHE	deletion	UNP Q9WXT2
B	?	-	MET	deletion	UNP Q9WXT2
C	-11	MET	-	initiating methionine	UNP Q9WXT2
C	-10	GLY	-	expression tag	UNP Q9WXT2
C	-9	SER	-	expression tag	UNP Q9WXT2
C	-8	ASP	-	expression tag	UNP Q9WXT2
C	-7	LYS	-	expression tag	UNP Q9WXT2
C	-6	ILE	-	expression tag	UNP Q9WXT2
C	-5	HIS	-	expression tag	UNP Q9WXT2
C	-4	HIS	-	expression tag	UNP Q9WXT2
C	-3	HIS	-	expression tag	UNP Q9WXT2
C	-2	HIS	-	expression tag	UNP Q9WXT2
C	-1	HIS	-	expression tag	UNP Q9WXT2
C	0	HIS	-	expression tag	UNP Q9WXT2
C	?	-	GLN	deletion	UNP Q9WXT2
C	?	-	GLY	deletion	UNP Q9WXT2
C	?	-	SER	deletion	UNP Q9WXT2
C	?	-	GLY	deletion	UNP Q9WXT2
C	?	-	TRP	deletion	UNP Q9WXT2
C	?	-	LEU	deletion	UNP Q9WXT2
C	?	-	LYS	deletion	UNP Q9WXT2
C	?	-	GLY	deletion	UNP Q9WXT2
C	?	-	ASP	deletion	UNP Q9WXT2
C	?	-	THR	deletion	UNP Q9WXT2
C	?	-	PRO	deletion	UNP Q9WXT2
C	?	-	ASP	deletion	UNP Q9WXT2
C	?	-	TYR	deletion	UNP Q9WXT2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PRO	deletion	UNP Q9WXT2
C	?	-	GLU	deletion	UNP Q9WXT2
C	?	-	GLY	deletion	UNP Q9WXT2
C	?	-	PRO	deletion	UNP Q9WXT2
C	?	-	VAL	deletion	UNP Q9WXT2
C	?	-	ASP	deletion	UNP Q9WXT2
C	?	-	PRO	deletion	UNP Q9WXT2
C	?	-	GLN	deletion	UNP Q9WXT2
C	?	-	TYR	deletion	UNP Q9WXT2
C	?	-	PRO	deletion	UNP Q9WXT2
C	?	-	GLY	deletion	UNP Q9WXT2
C	?	-	PHE	deletion	UNP Q9WXT2
C	?	-	MET	deletion	UNP Q9WXT2
D	-11	MET	-	initiating methionine	UNP Q9WXT2
D	-10	GLY	-	expression tag	UNP Q9WXT2
D	-9	SER	-	expression tag	UNP Q9WXT2
D	-8	ASP	-	expression tag	UNP Q9WXT2
D	-7	LYS	-	expression tag	UNP Q9WXT2
D	-6	ILE	-	expression tag	UNP Q9WXT2
D	-5	HIS	-	expression tag	UNP Q9WXT2
D	-4	HIS	-	expression tag	UNP Q9WXT2
D	-3	HIS	-	expression tag	UNP Q9WXT2
D	-2	HIS	-	expression tag	UNP Q9WXT2
D	-1	HIS	-	expression tag	UNP Q9WXT2
D	0	HIS	-	expression tag	UNP Q9WXT2
D	?	-	GLN	deletion	UNP Q9WXT2
D	?	-	GLY	deletion	UNP Q9WXT2
D	?	-	SER	deletion	UNP Q9WXT2
D	?	-	GLY	deletion	UNP Q9WXT2
D	?	-	TRP	deletion	UNP Q9WXT2
D	?	-	LEU	deletion	UNP Q9WXT2
D	?	-	LYS	deletion	UNP Q9WXT2
D	?	-	GLY	deletion	UNP Q9WXT2
D	?	-	ASP	deletion	UNP Q9WXT2
D	?	-	THR	deletion	UNP Q9WXT2
D	?	-	PRO	deletion	UNP Q9WXT2
D	?	-	ASP	deletion	UNP Q9WXT2
D	?	-	TYR	deletion	UNP Q9WXT2
D	?	-	PRO	deletion	UNP Q9WXT2
D	?	-	GLU	deletion	UNP Q9WXT2
D	?	-	GLY	deletion	UNP Q9WXT2
D	?	-	PRO	deletion	UNP Q9WXT2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	VAL	deletion	UNP Q9WXT2
D	?	-	ASP	deletion	UNP Q9WXT2
D	?	-	PRO	deletion	UNP Q9WXT2
D	?	-	GLN	deletion	UNP Q9WXT2
D	?	-	TYR	deletion	UNP Q9WXT2
D	?	-	PRO	deletion	UNP Q9WXT2
D	?	-	GLY	deletion	UNP Q9WXT2
D	?	-	PHE	deletion	UNP Q9WXT2
D	?	-	MET	deletion	UNP Q9WXT2
E	-11	MET	-	initiating methionine	UNP Q9WXT2
E	-10	GLY	-	expression tag	UNP Q9WXT2
E	-9	SER	-	expression tag	UNP Q9WXT2
E	-8	ASP	-	expression tag	UNP Q9WXT2
E	-7	LYS	-	expression tag	UNP Q9WXT2
E	-6	ILE	-	expression tag	UNP Q9WXT2
E	-5	HIS	-	expression tag	UNP Q9WXT2
E	-4	HIS	-	expression tag	UNP Q9WXT2
E	-3	HIS	-	expression tag	UNP Q9WXT2
E	-2	HIS	-	expression tag	UNP Q9WXT2
E	-1	HIS	-	expression tag	UNP Q9WXT2
E	0	HIS	-	expression tag	UNP Q9WXT2
E	?	-	GLN	deletion	UNP Q9WXT2
E	?	-	GLY	deletion	UNP Q9WXT2
E	?	-	SER	deletion	UNP Q9WXT2
E	?	-	GLY	deletion	UNP Q9WXT2
E	?	-	TRP	deletion	UNP Q9WXT2
E	?	-	LEU	deletion	UNP Q9WXT2
E	?	-	LYS	deletion	UNP Q9WXT2
E	?	-	GLY	deletion	UNP Q9WXT2
E	?	-	ASP	deletion	UNP Q9WXT2
E	?	-	THR	deletion	UNP Q9WXT2
E	?	-	PRO	deletion	UNP Q9WXT2
E	?	-	ASP	deletion	UNP Q9WXT2
E	?	-	TYR	deletion	UNP Q9WXT2
E	?	-	PRO	deletion	UNP Q9WXT2
E	?	-	GLU	deletion	UNP Q9WXT2
E	?	-	GLY	deletion	UNP Q9WXT2
E	?	-	PRO	deletion	UNP Q9WXT2
E	?	-	VAL	deletion	UNP Q9WXT2
E	?	-	ASP	deletion	UNP Q9WXT2
E	?	-	PRO	deletion	UNP Q9WXT2
E	?	-	GLN	deletion	UNP Q9WXT2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	TYR	deletion	UNP Q9WXT2
E	?	-	PRO	deletion	UNP Q9WXT2
E	?	-	GLY	deletion	UNP Q9WXT2
E	?	-	PHE	deletion	UNP Q9WXT2
E	?	-	MET	deletion	UNP Q9WXT2
F	-11	MET	-	initiating methionine	UNP Q9WXT2
F	-10	GLY	-	expression tag	UNP Q9WXT2
F	-9	SER	-	expression tag	UNP Q9WXT2
F	-8	ASP	-	expression tag	UNP Q9WXT2
F	-7	LYS	-	expression tag	UNP Q9WXT2
F	-6	ILE	-	expression tag	UNP Q9WXT2
F	-5	HIS	-	expression tag	UNP Q9WXT2
F	-4	HIS	-	expression tag	UNP Q9WXT2
F	-3	HIS	-	expression tag	UNP Q9WXT2
F	-2	HIS	-	expression tag	UNP Q9WXT2
F	-1	HIS	-	expression tag	UNP Q9WXT2
F	0	HIS	-	expression tag	UNP Q9WXT2
F	?	-	GLN	deletion	UNP Q9WXT2
F	?	-	GLY	deletion	UNP Q9WXT2
F	?	-	SER	deletion	UNP Q9WXT2
F	?	-	GLY	deletion	UNP Q9WXT2
F	?	-	TRP	deletion	UNP Q9WXT2
F	?	-	LEU	deletion	UNP Q9WXT2
F	?	-	LYS	deletion	UNP Q9WXT2
F	?	-	GLY	deletion	UNP Q9WXT2
F	?	-	ASP	deletion	UNP Q9WXT2
F	?	-	THR	deletion	UNP Q9WXT2
F	?	-	PRO	deletion	UNP Q9WXT2
F	?	-	ASP	deletion	UNP Q9WXT2
F	?	-	TYR	deletion	UNP Q9WXT2
F	?	-	PRO	deletion	UNP Q9WXT2
F	?	-	GLU	deletion	UNP Q9WXT2
F	?	-	GLY	deletion	UNP Q9WXT2
F	?	-	PRO	deletion	UNP Q9WXT2
F	?	-	VAL	deletion	UNP Q9WXT2
F	?	-	ASP	deletion	UNP Q9WXT2
F	?	-	PRO	deletion	UNP Q9WXT2
F	?	-	GLN	deletion	UNP Q9WXT2
F	?	-	TYR	deletion	UNP Q9WXT2
F	?	-	PRO	deletion	UNP Q9WXT2
F	?	-	GLY	deletion	UNP Q9WXT2
F	?	-	PHE	deletion	UNP Q9WXT2

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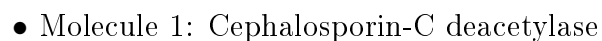
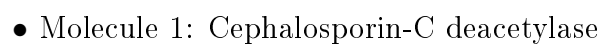
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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	MET	deletion	UNP Q9WXT2

- Molecule 2 is water.

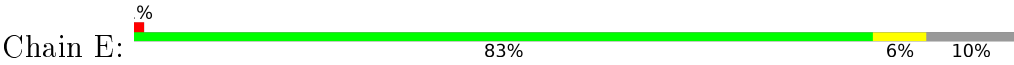
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total O 12 12	0	0
2	B	12	Total O 12 12	0	0
2	C	12	Total O 12 12	0	0
2	D	15	Total O 15 15	0	0
2	E	20	Total O 20 20	0	0
2	F	14	Total O 14 14	0	0

- Molecule 1: Cephalosporin-C deacetylase



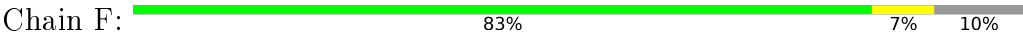
E323
LYS
GLY

• Molecule 1: Cephalosporin-C deacetylase



E240
D241
K242
P265
P282
H303
E323
LYS
GLY

• Molecule 1: Cephalosporin-C deacetylase



E239
E240
D241
K242
R248
P265
P292
H303
E313
E323
LYS
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.08Å 155.08Å 165.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.09 – 2.75 52.09 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.09-2.75) 99.9 (52.09-2.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.231 0.205 , 0.236	Depositor DCC
R_{free} test set	3028 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13326	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.96	0/2249	0.94	3/3057 (0.1%)
1	B	1.02	3/2263 (0.1%)	0.94	2/3076 (0.1%)
1	C	0.89	1/2262 (0.0%)	0.86	1/3076 (0.0%)
1	D	0.92	0/2269	0.90	2/3088 (0.1%)
1	E	1.04	3/2290 (0.1%)	0.94	4/3111 (0.1%)
1	F	1.00	3/2308 (0.1%)	0.99	11/3132 (0.4%)
All	All	0.97	10/13641 (0.1%)	0.93	23/18540 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	SER	CB-OG	-6.88	1.33	1.42
1	F	313	GLU	CD-OE2	-6.75	1.18	1.25
1	C	188	SER	CB-OG	-6.27	1.34	1.42
1	E	55	GLU	CD-OE1	5.97	1.32	1.25
1	F	180	GLU	CD-OE2	-5.75	1.19	1.25
1	B	156	TYR	CE1-CZ	5.66	1.46	1.38
1	E	156	TYR	CE1-CZ	5.48	1.45	1.38
1	B	80	GLU	CG-CD	5.47	1.60	1.51
1	F	156	TYR	CE1-CZ	5.31	1.45	1.38
1	E	188	SER	CB-OG	-5.26	1.35	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	241	ASP	CB-CG-OD1	8.94	126.35	118.30
1	A	241	ASP	CB-CG-OD1	8.83	126.25	118.30
1	D	241	ASP	CB-CG-OD1	8.61	126.05	118.30
1	C	241	ASP	CB-CG-OD1	8.39	125.85	118.30
1	E	241	ASP	CB-CG-OD1	8.23	125.71	118.30
1	B	241	ASP	CB-CG-OD1	7.73	125.26	118.30
1	F	118	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	F	180	GLU	CG-CD-OE1	6.93	132.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	248	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	E	47	MET	CG-SD-CE	6.76	111.01	100.20
1	F	231	GLU	OE1-CD-OE2	6.57	131.19	123.30
1	F	118	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	F	313	GLU	CG-CD-OE1	6.18	130.67	118.30
1	B	115	MET	CB-CG-SD	-6.14	93.99	112.40
1	F	218	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	E	96	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	F	159	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	15	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	F	180	GLU	CG-CD-OE2	-5.49	107.32	118.30
1	E	96	ARG	N-CA-CB	5.48	120.47	110.60
1	D	47	MET	CG-SD-CE	5.45	108.92	100.20
1	A	19	TYR	CG-CD2-CE2	-5.38	117.00	121.30
1	F	313	GLU	CG-CD-OE2	-5.36	107.58	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	A	2187	0	2067	6	0
1	B	2196	0	2086	8	0
1	C	2195	0	2079	8	0
1	D	2201	0	2069	7	0
1	E	2222	0	2107	10	0
1	F	2240	0	2150	8	0
2	A	12	0	0	1	0
2	B	12	0	0	0	0
2	C	12	0	0	0	0
2	D	15	0	0	0	0
2	E	20	0	0	0	0
2	F	14	0	0	0	0
All	All	13326	0	12558	43	0

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 2.

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:D:3:PHE:CD2	1:E:222:GLN:HB2	2.22	0.75
1:C:118:ARG:HH21	1:C:159:ARG:CB	2.06	0.67
1:D:188:SER:OG	1:D:303:HIS:NE2	2.43	0.51
1:A:188:SER:OG	1:A:303:HIS:NE2	2.45	0.49
1:C:188:SER:OG	1:C:303:HIS:NE2	2.45	0.49
1:F:188:SER:OG	1:F:303:HIS:NE2	2.46	0.48
1:D:3:PHE:CE2	1:E:222:GLN:HB2	2.50	0.46
1:E:81:GLU:OE1	1:E:81:GLU:N	2.48	0.46
1:B:115:MET:HE3	1:B:163:ASP:HB3	1.97	0.46
1:B:69:ILE:HG21	1:B:115:MET:HE1	1.99	0.45
1:B:188:SER:OG	1:B:303:HIS:NE2	2.50	0.44
1:A:213:PHE:CZ	1:A:228:PRO:HB2	2.52	0.44
1:D:265:PRO:HA	1:D:292:PRO:O	2.18	0.44
1:E:188:SER:OG	1:E:303:HIS:NE2	2.43	0.44
1:E:265:PRO:HA	1:E:292:PRO:O	2.19	0.43
1:E:57:TYR:HB2	1:E:73:LEU:HB3	2.00	0.43
1:E:3:PHE:CD2	1:F:222:GLN:HB2	2.54	0.43
1:B:239:HIS:HB3	1:B:242:LYS:HG3	2.00	0.43
1:E:239:HIS:HB3	1:E:242:LYS:HG3	2.00	0.43
1:F:239:HIS:HB3	1:F:242:LYS:HG3	2.01	0.43
1:F:265:PRO:HA	1:F:292:PRO:O	2.19	0.42
1:A:239:HIS:HB3	1:A:242:LYS:HG3	2.00	0.42
1:B:213:PHE:CZ	1:B:228:PRO:HB2	2.54	0.42
1:E:3:PHE:CE2	1:F:222:GLN:HB2	2.54	0.42
1:B:265:PRO:HA	1:B:292:PRO:O	2.19	0.42
1:B:227[A]:HIS:NE2	1:B:231:GLU:OE2	2.52	0.41
1:C:58:ASP:OD2	1:C:70:LYS:NZ	2.53	0.41
1:D:227[A]:HIS:NE2	1:D:231:GLU:OE2	2.54	0.41
1:A:47:MET:HE2	1:A:72:TRP:CE3	2.55	0.41
1:C:239:HIS:HB3	1:C:242:LYS:HG3	2.03	0.41
1:C:265:PRO:HA	1:C:292:PRO:O	2.21	0.41
1:F:227[A]:HIS:CG	1:F:228:PRO:HA	2.55	0.41
1:F:235:PHE:CE1	1:F:239:HIS:CD2	3.08	0.41
1:E:227[A]:HIS:NE2	1:E:231:GLU:OE2	2.54	0.41
1:D:239:HIS:HB3	1:D:242:LYS:HG3	2.03	0.41
1:B:61:PHE:HZ	1:B:115:MET:HE1	1.84	0.41
1:C:278:PRO:HA	1:C:279:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:PHE:CZ	1:C:228:PRO:HB2	2.56	0.41
1:D:227[A]:HIS:CG	1:D:228:PRO:HA	2.56	0.40
1:A:265:PRO:HA	1:A:292:PRO:O	2.22	0.40
1:A:218:ARG:HG2	2:A:402:HOH:O	2.21	0.40
1:F:188:SER:HB3	1:F:189:GLN:H	1.62	0.40
1:C:227[A]:HIS:NE2	1:C:231:GLU:OE2	2.55	0.40

There are no symmetry-related clashes.

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	A	274/311 (88%)	264 (96%)	9 (3%)	1 (0%)	39	72
1	B	273/311 (88%)	267 (98%)	6 (2%)	0	100	100
1	C	274/311 (88%)	265 (97%)	8 (3%)	1 (0%)	39	72
1	D	278/311 (89%)	267 (96%)	10 (4%)	1 (0%)	39	72
1	E	274/311 (88%)	266 (97%)	7 (3%)	1 (0%)	39	72
1	F	274/311 (88%)	268 (98%)	5 (2%)	1 (0%)	39	72
All	All	1647/1866 (88%)	1597 (97%)	45 (3%)	5 (0%)	46	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	97	GLY
1	F	97	GLY
1	A	97	GLY
1	D	97	GLY
1	C	97	GLY

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	217/264 (82%)	216 (100%)	1 (0%)	92	97
1	B	221/264 (84%)	217 (98%)	4 (2%)	66	90
1	C	220/264 (83%)	219 (100%)	1 (0%)	92	97
1	D	217/264 (82%)	216 (100%)	1 (0%)	92	97
1	E	225/264 (85%)	224 (100%)	1 (0%)	93	98
1	F	230/264 (87%)	228 (99%)	2 (1%)	84	95
All	All	1330/1584 (84%)	1320 (99%)	10 (1%)	86	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	VAL
1	B	96	ARG
1	B	115	MET
1	B	221	VAL
1	B	238	THR
1	C	221	VAL
1	D	221	VAL
1	E	221	VAL
1	F	118	ARG
1	F	221	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	100	HIS
1	F	239	HIS

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

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	280/311 (90%)	-0.07	1 (0%) 93 92	34, 49, 81, 99	0
1	B	278/311 (89%)	-0.11	0 100 100	37, 50, 72, 94	0
1	C	279/311 (89%)	0.13	7 (2%) 61 54	39, 60, 89, 109	0
1	D	283/311 (90%)	-0.04	3 (1%) 82 78	30, 56, 87, 102	0
1	E	279/311 (89%)	-0.08	2 (0%) 89 86	34, 44, 65, 85	0
1	F	279/311 (89%)	0.02	1 (0%) 93 92	34, 49, 77, 93	0
All	All	1678/1866 (89%)	-0.02	14 (0%) 87 83	30, 51, 81, 109	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	157	TYR	3.2
1	E	2	ALA	2.7
1	D	-2	HIS	2.7
1	D	156	TYR	2.6
1	C	157	TYR	2.5
1	C	27	PHE	2.4
1	C	24	PHE	2.3
1	E	156	TYR	2.3
1	A	2	ALA	2.3
1	C	65	ARG	2.2
1	C	69	ILE	2.1
1	C	63	GLY	2.1
1	F	67	GLN	2.0
1	C	32	LEU	2.0

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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.