



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:52 pm BST

PDB ID : 3T3W  
Title : Crystal structure of probable enoyl-CoA hydratase from mycobacterium thermoresistibile  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2011-07-25  
Resolution : 1.80 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

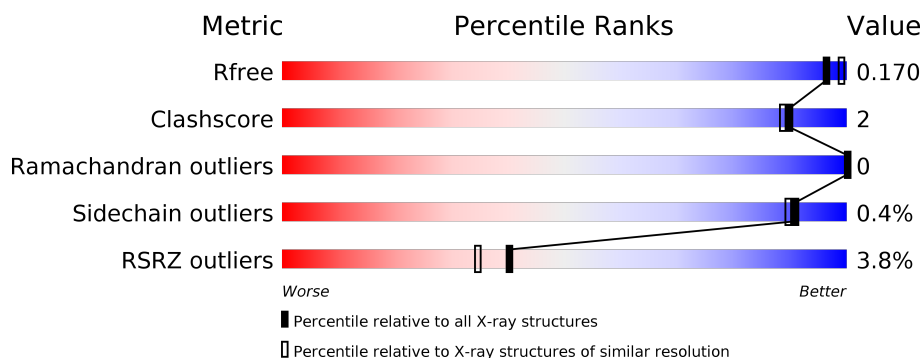
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	279	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	279	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	279	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>• •</div> <div>12%</div> </div> </div>
1	D	279	<div> <div>0%</div> <div> <div></div> <div>84%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	279	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>5% •</div> <div>12%</div> </div> </div>
1	F	279	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>5%</div> <div>11%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TRS	A	302	-	X	-	-
4	TRS	B	302	-	X	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12707 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 Enoyl-CoA hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	5	0
			1869	1178	331	351	9			
1	B	237	Total	C	N	O	S	0	5	0
			1840	1157	329	346	8			
1	C	246	Total	C	N	O	S	0	5	0
			1917	1206	344	359	8			
1	D	247	Total	C	N	O	S	0	3	0
			1919	1212	340	357	10			
1	E	246	Total	C	N	O	S	0	5	0
			1928	1215	343	361	9			
1	F	248	Total	C	N	O	S	0	6	0
			1927	1211	342	365	9			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP G7CL68
A	-1	SER	-	EXPRESSION TAG	UNP G7CL68
A	0	MET	-	EXPRESSION TAG	UNP G7CL68
A	1	VAL	-	EXPRESSION TAG	UNP G7CL68
A	2	ALA	-	EXPRESSION TAG	UNP G7CL68
A	3	PRO	-	EXPRESSION TAG	UNP G7CL68
A	4	SER	-	EXPRESSION TAG	UNP G7CL68
A	5	TRP	-	EXPRESSION TAG	UNP G7CL68
A	6	ARG	-	EXPRESSION TAG	UNP G7CL68
A	7	ARG	-	EXPRESSION TAG	UNP G7CL68
A	8	PRO	-	EXPRESSION TAG	UNP G7CL68
A	9	SER	-	EXPRESSION TAG	UNP G7CL68
A	10	ARG	-	EXPRESSION TAG	UNP G7CL68
A	11	PRO	-	EXPRESSION TAG	UNP G7CL68
A	12	GLU	-	EXPRESSION TAG	UNP G7CL68
A	13	GLN	-	EXPRESSION TAG	UNP G7CL68
A	14	ARG	-	EXPRESSION TAG	UNP G7CL68

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	THR	-	EXPRESSION TAG	UNP G7CL68
A	16	GLU	-	EXPRESSION TAG	UNP G7CL68
A	155	ASP	GLY	CONFLICT	UNP G7CL68
B	-2	GLY	-	EXPRESSION TAG	UNP G7CL68
B	-1	SER	-	EXPRESSION TAG	UNP G7CL68
B	0	MET	-	EXPRESSION TAG	UNP G7CL68
B	1	VAL	-	EXPRESSION TAG	UNP G7CL68
B	2	ALA	-	EXPRESSION TAG	UNP G7CL68
B	3	PRO	-	EXPRESSION TAG	UNP G7CL68
B	4	SER	-	EXPRESSION TAG	UNP G7CL68
B	5	TRP	-	EXPRESSION TAG	UNP G7CL68
B	6	ARG	-	EXPRESSION TAG	UNP G7CL68
B	7	ARG	-	EXPRESSION TAG	UNP G7CL68
B	8	PRO	-	EXPRESSION TAG	UNP G7CL68
B	9	SER	-	EXPRESSION TAG	UNP G7CL68
B	10	ARG	-	EXPRESSION TAG	UNP G7CL68
B	11	PRO	-	EXPRESSION TAG	UNP G7CL68
B	12	GLU	-	EXPRESSION TAG	UNP G7CL68
B	13	GLN	-	EXPRESSION TAG	UNP G7CL68
B	14	ARG	-	EXPRESSION TAG	UNP G7CL68
B	15	THR	-	EXPRESSION TAG	UNP G7CL68
B	16	GLU	-	EXPRESSION TAG	UNP G7CL68
B	155	ASP	GLY	CONFLICT	UNP G7CL68
C	-2	GLY	-	EXPRESSION TAG	UNP G7CL68
C	-1	SER	-	EXPRESSION TAG	UNP G7CL68
C	0	MET	-	EXPRESSION TAG	UNP G7CL68
C	1	VAL	-	EXPRESSION TAG	UNP G7CL68
C	2	ALA	-	EXPRESSION TAG	UNP G7CL68
C	3	PRO	-	EXPRESSION TAG	UNP G7CL68
C	4	SER	-	EXPRESSION TAG	UNP G7CL68
C	5	TRP	-	EXPRESSION TAG	UNP G7CL68
C	6	ARG	-	EXPRESSION TAG	UNP G7CL68
C	7	ARG	-	EXPRESSION TAG	UNP G7CL68
C	8	PRO	-	EXPRESSION TAG	UNP G7CL68
C	9	SER	-	EXPRESSION TAG	UNP G7CL68
C	10	ARG	-	EXPRESSION TAG	UNP G7CL68
C	11	PRO	-	EXPRESSION TAG	UNP G7CL68
C	12	GLU	-	EXPRESSION TAG	UNP G7CL68
C	13	GLN	-	EXPRESSION TAG	UNP G7CL68
C	14	ARG	-	EXPRESSION TAG	UNP G7CL68
C	15	THR	-	EXPRESSION TAG	UNP G7CL68
C	16	GLU	-	EXPRESSION TAG	UNP G7CL68

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Chain	Residue	Modelled	Actual	Comment	Reference
C	155	ASP	GLY	CONFLICT	UNP G7CL68
D	-2	GLY	-	EXPRESSION TAG	UNP G7CL68
D	-1	SER	-	EXPRESSION TAG	UNP G7CL68
D	0	MET	-	EXPRESSION TAG	UNP G7CL68
D	1	VAL	-	EXPRESSION TAG	UNP G7CL68
D	2	ALA	-	EXPRESSION TAG	UNP G7CL68
D	3	PRO	-	EXPRESSION TAG	UNP G7CL68
D	4	SER	-	EXPRESSION TAG	UNP G7CL68
D	5	TRP	-	EXPRESSION TAG	UNP G7CL68
D	6	ARG	-	EXPRESSION TAG	UNP G7CL68
D	7	ARG	-	EXPRESSION TAG	UNP G7CL68
D	8	PRO	-	EXPRESSION TAG	UNP G7CL68
D	9	SER	-	EXPRESSION TAG	UNP G7CL68
D	10	ARG	-	EXPRESSION TAG	UNP G7CL68
D	11	PRO	-	EXPRESSION TAG	UNP G7CL68
D	12	GLU	-	EXPRESSION TAG	UNP G7CL68
D	13	GLN	-	EXPRESSION TAG	UNP G7CL68
D	14	ARG	-	EXPRESSION TAG	UNP G7CL68
D	15	THR	-	EXPRESSION TAG	UNP G7CL68
D	16	GLU	-	EXPRESSION TAG	UNP G7CL68
D	155	ASP	GLY	CONFLICT	UNP G7CL68
E	-2	GLY	-	EXPRESSION TAG	UNP G7CL68
E	-1	SER	-	EXPRESSION TAG	UNP G7CL68
E	0	MET	-	EXPRESSION TAG	UNP G7CL68
E	1	VAL	-	EXPRESSION TAG	UNP G7CL68
E	2	ALA	-	EXPRESSION TAG	UNP G7CL68
E	3	PRO	-	EXPRESSION TAG	UNP G7CL68
E	4	SER	-	EXPRESSION TAG	UNP G7CL68
E	5	TRP	-	EXPRESSION TAG	UNP G7CL68
E	6	ARG	-	EXPRESSION TAG	UNP G7CL68
E	7	ARG	-	EXPRESSION TAG	UNP G7CL68
E	8	PRO	-	EXPRESSION TAG	UNP G7CL68
E	9	SER	-	EXPRESSION TAG	UNP G7CL68
E	10	ARG	-	EXPRESSION TAG	UNP G7CL68
E	11	PRO	-	EXPRESSION TAG	UNP G7CL68
E	12	GLU	-	EXPRESSION TAG	UNP G7CL68
E	13	GLN	-	EXPRESSION TAG	UNP G7CL68
E	14	ARG	-	EXPRESSION TAG	UNP G7CL68
E	15	THR	-	EXPRESSION TAG	UNP G7CL68
E	16	GLU	-	EXPRESSION TAG	UNP G7CL68
E	155	ASP	GLY	CONFLICT	UNP G7CL68
F	-2	GLY	-	EXPRESSION TAG	UNP G7CL68

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	SER	-	EXPRESSION TAG	UNP G7CL68
F	0	MET	-	EXPRESSION TAG	UNP G7CL68
F	1	VAL	-	EXPRESSION TAG	UNP G7CL68
F	2	ALA	-	EXPRESSION TAG	UNP G7CL68
F	3	PRO	-	EXPRESSION TAG	UNP G7CL68
F	4	SER	-	EXPRESSION TAG	UNP G7CL68
F	5	TRP	-	EXPRESSION TAG	UNP G7CL68
F	6	ARG	-	EXPRESSION TAG	UNP G7CL68
F	7	ARG	-	EXPRESSION TAG	UNP G7CL68
F	8	PRO	-	EXPRESSION TAG	UNP G7CL68
F	9	SER	-	EXPRESSION TAG	UNP G7CL68
F	10	ARG	-	EXPRESSION TAG	UNP G7CL68
F	11	PRO	-	EXPRESSION TAG	UNP G7CL68
F	12	GLU	-	EXPRESSION TAG	UNP G7CL68
F	13	GLN	-	EXPRESSION TAG	UNP G7CL68
F	14	ARG	-	EXPRESSION TAG	UNP G7CL68
F	15	THR	-	EXPRESSION TAG	UNP G7CL68
F	16	GLU	-	EXPRESSION TAG	UNP G7CL68
F	155	ASP	GLY	CONFLICT	UNP G7CL68

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

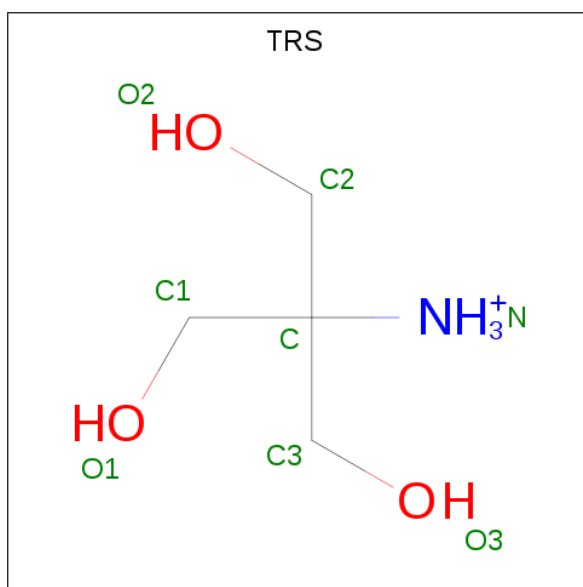
- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	I	0	0
			1	1		
5	E	1	Total	I	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	191	Total	O	0	0
			191	191		
6	B	192	Total	O	0	0
			192	192		
6	C	228	Total	O	0	0
			228	228		
6	D	219	Total	O	0	0
			219	219		
6	E	222	Total	O	0	0
			222	222		

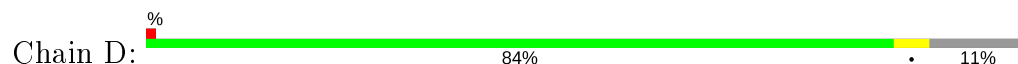
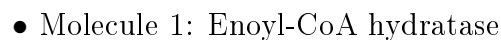
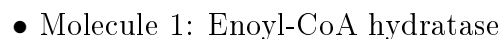
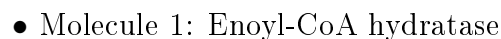
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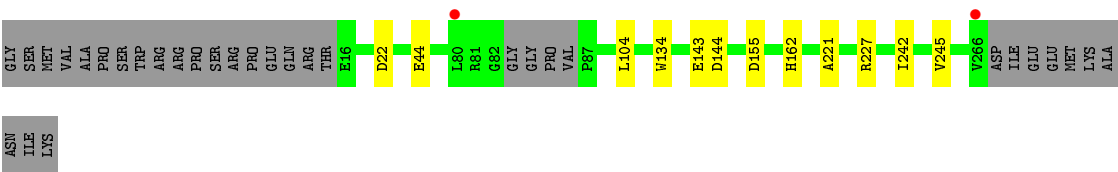
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	203	Total 203	O 203	0	0

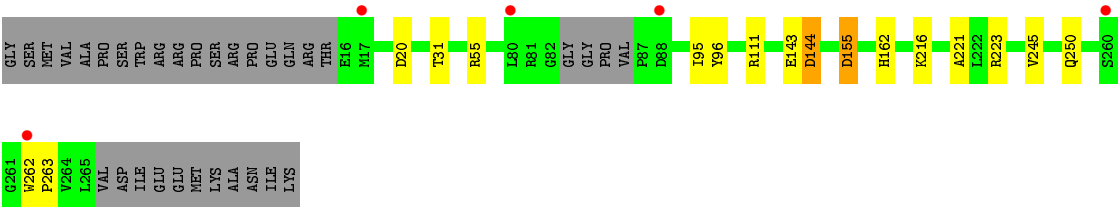
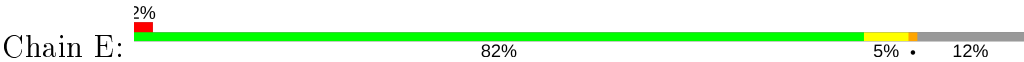


- Molecule 1: Enoyl-CoA hydratase

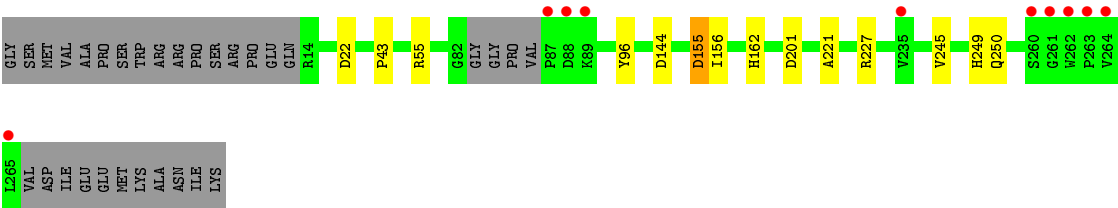
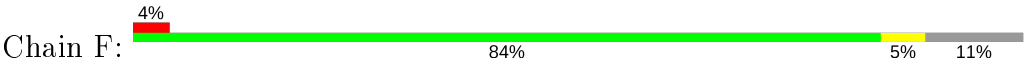




● Molecule 1: Enoyl-CoA hydratase



● Molecule 1: Enoyl-CoA hydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.24Å 124.24Å 212.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.22 – 1.80 49.22 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.22-1.80) 99.7 (49.22-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.28 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.139 , 0.165 0.146 , 0.170	Depositor DCC
$R_{free}$ test set	7676 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12707	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IOD, TRS, EDO

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	0.74	0/1922	0.79	1/2614 (0.0%)
1	B	0.74	0/1888	0.75	1/2568 (0.0%)
1	C	0.73	0/1971	0.77	2/2678 (0.1%)
1	D	0.78	2/1969 (0.1%)	0.84	4/2678 (0.1%)
1	E	0.78	3/1982 (0.2%)	0.92	7/2695 (0.3%)
1	F	0.75	0/1985	0.86	6/2700 (0.2%)
All	All	0.75	5/11717 (0.0%)	0.83	21/15933 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	262	TRP	CD2-CE2	5.60	1.48	1.41
1	E	144[A]	ASP	CB-CG	5.50	1.63	1.51
1	E	144[B]	ASP	CB-CG	5.50	1.63	1.51
1	D	134	TRP	CD2-CE2	5.19	1.47	1.41
1	D	144	ASP	CB-CG	5.09	1.62	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	144[A]	ASP	CB-CG-OD1	13.00	130.00	118.30
1	E	144[B]	ASP	CB-CG-OD1	13.00	130.00	118.30
1	F	55	ARG	NE-CZ-NH2	10.46	125.53	120.30
1	D	144	ASP	CB-CG-OD2	10.25	127.53	118.30
1	F	144	ASP	CB-CG-OD2	9.57	126.91	118.30
1	E	55	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	D	22	ASP	CB-CG-OD2	8.14	125.63	118.30
1	A	144	ASP	CB-CG-OD2	7.98	125.48	118.30
1	F	55	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	E	223	ARG	NE-CZ-NH1	-7.48	116.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	55	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	D	227	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	F	22	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	172	LYS	CD-CE-NZ	5.89	125.24	111.70
1	C	144	ASP	CB-CG-OD2	5.84	123.56	118.30
1	E	155	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	223	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	D	44	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	E	111	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	F	201	ASP	CB-CG-OD1	5.04	122.83	118.30
1	F	227	ARG	NE-CZ-NH1	5.03	122.82	120.30

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	1869	0	1821	8	0
1	B	1840	0	1784	7	0
1	C	1917	0	1875	7	0
1	D	1919	0	1878	5	0
1	E	1928	0	1876	12	0
1	F	1927	0	1864	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	4	0	6	1	0
3	D	4	0	6	0	0
3	E	4	0	6	0	0
3	F	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	8	0	12	0	0
4	B	8	0	12	0	0
5	E	1	0	0	0	0
5	F	1	0	0	1	0
6	A	191	0	0	2	0
6	B	192	0	0	1	0
6	C	228	0	0	0	0
6	D	219	0	0	1	0
6	E	222	0	0	4	0
6	F	203	0	0	1	0
All	All	12707	0	11164	40	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 (40) 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:E:216:LYS:CE	6:E:1191:HOH:O	2.32	0.76
1:C:95:ILE:HD13	1:C:263:PRO:HB3	1.77	0.65
1:E:216:LYS:HE3	6:E:1191:HOH:O	1.98	0.63
1:A:155[B]:ASP:HA	1:F:221:ALA:HB2	1.81	0.61
1:B:143:GLU:OE2	6:B:970:HOH:O	2.17	0.61
1:F:155[B]:ASP:CG	6:F:1194:HOH:O	2.38	0.60
1:A:155[A]:ASP:HA	1:F:221:ALA:HB2	1.83	0.59
1:E:143:GLU:OE2	6:E:1254:HOH:O	2.18	0.56
1:E:95:ILE:HD11	1:E:263:PRO:HG3	1.86	0.56
1:B:155:ASP:HA	1:D:221:ALA:HB2	1.90	0.54
1:B:156:ILE:HG21	1:B:249:HIS:CE1	2.43	0.54
1:D:143:GLU:OE2	6:D:339:HOH:O	2.18	0.53
1:C:156:ILE:HG21	1:C:249:HIS:CE1	2.46	0.51
1:B:221:ALA:HB2	1:C:155:ASP:HA	1.93	0.51
1:E:216:LYS:HE2	6:E:1191:HOH:O	2.02	0.51
1:F:156:ILE:HG21	1:F:249:HIS:CE1	2.46	0.50
1:E:221:ALA:HB2	1:F:155[A]:ASP:HA	1.94	0.49
1:A:95:ILE:HD13	1:A:263:PRO:HB3	1.94	0.48
1:C:171:ARG:CZ	3:C:303:EDO:H12	2.43	0.48
1:A:221:ALA:HB2	1:E:155:ASP:HA	1.96	0.47
1:F:43:PRO:HD2	5:F:310:IOD:I	2.85	0.46
1:A:143:GLU:OE2	6:A:890:HOH:O	2.20	0.46
1:E:20[B]:ASP:HB3	1:E:31:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:HIS:HB2	1:F:245:VAL:HG11	1.96	0.46
1:E:221:ALA:HB2	1:F:155[B]:ASP:HA	1.97	0.45
1:A:156:ILE:HG21	1:A:249:HIS:CE1	2.52	0.45
1:A:172:LYS:HE2	6:A:900:HOH:O	2.18	0.43
1:C:162:HIS:HB2	1:C:245:VAL:HG11	2.01	0.43
1:B:96:TYR:CD1	1:B:250:GLN:HG3	2.54	0.42
1:B:166:TRP:CZ2	1:B:238:PHE:HA	2.54	0.42
1:D:162:HIS:HB2	1:D:245:VAL:HG11	2.01	0.42
1:C:221:ALA:HB2	1:D:155:ASP:HA	2.00	0.42
1:C:96:TYR:CD1	1:C:250:GLN:HG3	2.54	0.42
1:A:198:VAL:HG11	1:A:206[B]:GLU:HG2	2.01	0.42
1:E:162:HIS:HB2	1:E:245:VAL:HG11	2.02	0.41
1:F:96:TYR:CD1	1:F:250:GLN:HG3	2.55	0.41
1:B:162:HIS:HB2	1:B:245:VAL:HG11	2.03	0.41
1:E:96:TYR:CD1	1:E:250:GLN:HG3	2.55	0.41
1:E:95:ILE:HD13	1:E:263:PRO:HB3	2.03	0.40
1:D:104:LEU:HD11	1:D:242:ILE:HG22	2.02	0.40

There are no symmetry-related clashes.

## 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	242/279 (87%)	232 (96%)	10 (4%)	0	100	100
1	B	238/279 (85%)	229 (96%)	9 (4%)	0	100	100
1	C	247/279 (88%)	238 (96%)	9 (4%)	0	100	100
1	D	246/279 (88%)	237 (96%)	9 (4%)	0	100	100
1	E	247/279 (88%)	238 (96%)	9 (4%)	0	100	100
1	F	250/279 (90%)	239 (96%)	11 (4%)	0	100	100
All	All	1470/1674 (88%)	1413 (96%)	57 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	192/227 (85%)	192 (100%)	0	100	100
1	B	187/227 (82%)	186 (100%)	1 (0%)	88	87
1	C	197/227 (87%)	195 (99%)	2 (1%)	76	71
1	D	198/227 (87%)	198 (100%)	0	100	100
1	E	199/227 (88%)	197 (99%)	2 (1%)	76	71
1	F	198/227 (87%)	196 (99%)	2 (1%)	76	71
All	All	1171/1362 (86%)	1164 (99%)	7 (1%)	91	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	155	ASP
1	C	155	ASP
1	C	263	PRO
1	E	144[A]	ASP
1	E	144[B]	ASP
1	F	155[A]	ASP
1	F	155[B]	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	98	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](#)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 for Mogul analysis.

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	$\# Z  > 2$
3	EDO	E	303	-	3,3,3	0.45	0	2,2,2	0.55	0
3	EDO	A	303	-	3,3,3	0.42	0	2,2,2	0.46	0
4	TRS	A	302	-	7,7,7	0.40	0	9,9,9	4.18	7 (77%)
3	EDO	F	304	-	3,3,3	0.56	0	2,2,2	0.12	0
3	EDO	D	303	-	3,3,3	0.47	0	2,2,2	0.40	0
3	EDO	F	303	-	3,3,3	0.37	0	2,2,2	0.50	0
4	TRS	B	302	-	7,7,7	0.49	0	9,9,9	4.21	6 (66%)
3	EDO	B	303	-	3,3,3	0.35	0	2,2,2	0.74	0
3	EDO	C	303	-	3,3,3	0.30	0	2,2,2	0.88	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
3	EDO	E	303	-	-	0/1/1/1	-
3	EDO	A	303	-	-	0/1/1/1	-
4	TRS	A	302	-	-	6/9/9/9	-
3	EDO	F	304	-	-	0/1/1/1	-
3	EDO	D	303	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	F	303	-	-	0/1/1/1	-
4	TRS	B	302	-	-	5/9/9/9	-
3	EDO	B	303	-	-	0/1/1/1	-
3	EDO	C	303	-	-	1/1/1/1	-

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	TRS	C2-C-N	-6.93	87.29	107.98
4	B	302	TRS	C2-C-N	-6.69	88.01	107.98
4	B	302	TRS	C3-C-N	-6.64	88.15	107.98
4	A	302	TRS	C1-C-N	-6.53	88.48	107.98
4	B	302	TRS	C1-C-N	-6.42	88.82	107.98
4	A	302	TRS	C3-C-N	-5.75	90.82	107.98
4	A	302	TRS	C2-C-C1	3.62	122.03	110.81
4	B	302	TRS	C3-C-C2	3.15	120.58	110.81
4	B	302	TRS	C2-C-C1	2.97	120.01	110.81
4	A	302	TRS	C3-C-C2	2.84	119.60	110.81
4	B	302	TRS	C3-C-C1	2.69	119.15	110.81
4	A	302	TRS	C3-C-C1	2.40	118.25	110.81
4	A	302	TRS	O1-C1-C	-2.04	104.53	111.00

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	TRS	C3-C-C1-O1
4	B	302	TRS	C1-C-C2-O2
4	B	302	TRS	N-C-C2-O2
4	B	302	TRS	C2-C-C3-O3
4	B	302	TRS	N-C-C3-O3
4	A	302	TRS	C3-C-C1-O1
4	A	302	TRS	N-C-C1-O1
4	A	302	TRS	C1-C-C2-O2
4	A	302	TRS	N-C-C2-O2
4	A	302	TRS	C2-C-C3-O3
4	A	302	TRS	N-C-C3-O3
3	C	303	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	303	EDO	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	241/279 (86%)	-0.05	16 (6%)	18 14	6, 13, 31, 52	0
1	B	237/279 (84%)	-0.12	11 (4%)	32 26	6, 13, 30, 53	0
1	C	246/279 (88%)	-0.27	11 (4%)	33 27	6, 12, 29, 54	0
1	D	247/279 (88%)	-0.35	2 (0%)	86 84	6, 12, 25, 51	0
1	E	246/279 (88%)	-0.34	5 (2%)	65 61	6, 10, 26, 48	0
1	F	248/279 (88%)	-0.29	10 (4%)	38 32	6, 12, 28, 55	0
All	All	1465/1674 (87%)	-0.23	55 (3%)	40 35	6, 12, 29, 55	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	80	LEU	7.9
1	F	262	TRP	7.4
1	A	262	TRP	6.7
1	A	259	VAL	6.4
1	A	260	SER	5.4
1	E	262	TRP	5.3
1	A	264	VAL	5.1
1	F	264	VAL	4.9
1	B	259	VAL	4.7
1	A	261	GLY	4.6
1	B	90	LEU	4.5
1	A	90	LEU	4.4
1	A	80	LEU	4.2
1	C	262	TRP	4.1
1	B	260	SER	4.0
1	F	265	LEU	3.8
1	F	261	GLY	3.7
1	B	16	GLU	3.7
1	B	94	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	263	PRO	3.5
1	C	264	VAL	3.4
1	C	88	ASP	3.4
1	A	257	MET	3.4
1	F	260	SER	3.3
1	C	265	LEU	3.3
1	C	17	MET	3.3
1	B	81	ARG	3.2
1	B	17	MET	3.2
1	F	263	PRO	3.2
1	C	260	SER	3.1
1	E	80	LEU	3.0
1	E	88	ASP	3.0
1	F	88	ASP	3.0
1	C	80	LEU	2.9
1	A	256	ALA	2.9
1	A	81	ARG	2.7
1	A	16	GLU	2.6
1	B	258	SER	2.6
1	A	17	MET	2.6
1	F	89	LYS	2.5
1	C	87	PRO	2.5
1	A	258	SER	2.5
1	F	87	PRO	2.4
1	B	257	MET	2.4
1	A	91	THR	2.2
1	C	261	GLY	2.2
1	E	17	MET	2.2
1	B	91	THR	2.2
1	A	235	VAL	2.1
1	D	266	VAL	2.1
1	C	89	LYS	2.1
1	D	80	LEU	2.1
1	C	235	VAL	2.1
1	E	260	SER	2.1
1	F	235	VAL	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 ⓘ

There are no carbohydrates in this entry.

### 6.4 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	TRS	B	302	8/8	0.85	0.16	32,35,37,38	0
4	TRS	A	302	8/8	0.87	0.15	32,33,34,34	0
3	EDO	B	303	4/4	0.91	0.13	18,21,21,22	0
3	EDO	C	303	4/4	0.93	0.09	20,22,23,25	0
5	IOD	F	310	1/1	0.95	0.22	53,53,53,53	0
3	EDO	E	303	4/4	0.96	0.15	16,19,19,22	0
3	EDO	F	304	4/4	0.96	0.11	25,27,27,29	0
3	EDO	D	303	4/4	0.96	0.10	20,22,23,24	0
3	EDO	F	303	4/4	0.97	0.09	16,16,17,18	0
3	EDO	A	303	4/4	0.97	0.11	17,20,21,24	0
5	IOD	E	310	1/1	0.98	0.25	64,64,64,64	0
2	ZN	F	301	1/1	1.00	0.03	11,11,11,11	0
2	ZN	B	301	1/1	1.00	0.09	18,18,18,18	0
2	ZN	E	301	1/1	1.00	0.03	10,10,10,10	0
2	ZN	D	301	1/1	1.00	0.04	10,10,10,10	0
2	ZN	C	301	1/1	1.00	0.02	11,11,11,11	0
2	ZN	A	301	1/1	1.00	0.10	18,18,18,18	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.