



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:27 AM UTC

PDB ID : 5LFM / pdb\_00005lfm  
Title : MamA RS-1 Ars<sup>TM</sup> double mutant  
Authors : Zarivach, R.; Cronin, S.L.  
Deposited on : 2016-07-03  
Resolution : 3.28 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
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

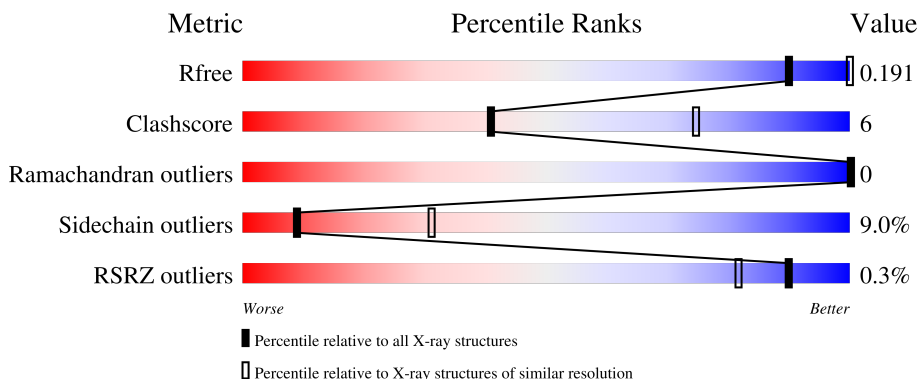
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.28 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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 of 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	202	 73% 13% • 12%
1	B	202	 75% 10% • 13%
1	C	202	 73% 11% • 13%
1	D	202	 76% 9% • 13%
1	E	202	 72% 12% • 12%

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Mol	Chain	Length	Quality of chain
1	F	202	 75% 10% • 12%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8563 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 Magnetosome protein MamA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	177	1423	905	255	256	7	0	0	0
1	B	176	1417	902	254	254	7	0	0	0
1	C	176	1417	902	254	254	7	0	0	0
1	D	176	1417	902	254	254	7	0	0	0
1	E	177	1423	905	255	256	7	0	0	0
1	F	178	1431	909	256	259	7	0	0	0

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	initiating methionine	UNP C4XPQ7
A	38	ALA	-	expression tag	UNP C4XPQ7
A	39	MET	-	expression tag	UNP C4XPQ7
A	40	GLY	-	expression tag	UNP C4XPQ7
A	46	PHE	TYR	conflict	UNP C4XPQ7
A	65	PHE	TYR	conflict	UNP C4XPQ7
A	68	LEU	GLU	conflict	UNP C4XPQ7
A	124	ILE	MET	conflict	UNP C4XPQ7
A	140	ALA	GLU	conflict	UNP C4XPQ7
A	141	ALA	LYS	conflict	UNP C4XPQ7
A	143	ALA	GLU	conflict	UNP C4XPQ7
A	218	GLU	-	expression tag	UNP C4XPQ7
A	219	LEU	-	expression tag	UNP C4XPQ7
A	220	ALA	-	expression tag	UNP C4XPQ7
A	221	LEU	-	expression tag	UNP C4XPQ7
A	222	VAL	-	expression tag	UNP C4XPQ7
A	223	PRO	-	expression tag	UNP C4XPQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	224	ARG	-	expression tag	UNP C4XPQ7
A	225	GLY	-	expression tag	UNP C4XPQ7
A	226	SER	-	expression tag	UNP C4XPQ7
A	227	SER	-	expression tag	UNP C4XPQ7
A	228	ALA	-	expression tag	UNP C4XPQ7
A	229	HIS	-	expression tag	UNP C4XPQ7
A	230	HIS	-	expression tag	UNP C4XPQ7
A	231	HIS	-	expression tag	UNP C4XPQ7
A	232	HIS	-	expression tag	UNP C4XPQ7
A	233	HIS	-	expression tag	UNP C4XPQ7
A	234	HIS	-	expression tag	UNP C4XPQ7
A	235	HIS	-	expression tag	UNP C4XPQ7
A	236	HIS	-	expression tag	UNP C4XPQ7
A	237	HIS	-	expression tag	UNP C4XPQ7
A	238	HIS	-	expression tag	UNP C4XPQ7
B	37	MET	-	initiating methionine	UNP C4XPQ7
B	38	ALA	-	expression tag	UNP C4XPQ7
B	39	MET	-	expression tag	UNP C4XPQ7
B	40	GLY	-	expression tag	UNP C4XPQ7
B	46	PHE	TYR	conflict	UNP C4XPQ7
B	65	PHE	TYR	conflict	UNP C4XPQ7
B	68	LEU	GLU	conflict	UNP C4XPQ7
B	124	ILE	MET	conflict	UNP C4XPQ7
B	140	ALA	GLU	conflict	UNP C4XPQ7
B	141	ALA	LYS	conflict	UNP C4XPQ7
B	143	ALA	GLU	conflict	UNP C4XPQ7
B	218	GLU	-	expression tag	UNP C4XPQ7
B	219	LEU	-	expression tag	UNP C4XPQ7
B	220	ALA	-	expression tag	UNP C4XPQ7
B	221	LEU	-	expression tag	UNP C4XPQ7
B	222	VAL	-	expression tag	UNP C4XPQ7
B	223	PRO	-	expression tag	UNP C4XPQ7
B	224	ARG	-	expression tag	UNP C4XPQ7
B	225	GLY	-	expression tag	UNP C4XPQ7
B	226	SER	-	expression tag	UNP C4XPQ7
B	227	SER	-	expression tag	UNP C4XPQ7
B	228	ALA	-	expression tag	UNP C4XPQ7
B	229	HIS	-	expression tag	UNP C4XPQ7
B	230	HIS	-	expression tag	UNP C4XPQ7
B	231	HIS	-	expression tag	UNP C4XPQ7
B	232	HIS	-	expression tag	UNP C4XPQ7
B	233	HIS	-	expression tag	UNP C4XPQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	234	HIS	-	expression tag	UNP C4XPQ7
B	235	HIS	-	expression tag	UNP C4XPQ7
B	236	HIS	-	expression tag	UNP C4XPQ7
B	237	HIS	-	expression tag	UNP C4XPQ7
B	238	HIS	-	expression tag	UNP C4XPQ7
C	37	MET	-	initiating methionine	UNP C4XPQ7
C	38	ALA	-	expression tag	UNP C4XPQ7
C	39	MET	-	expression tag	UNP C4XPQ7
C	40	GLY	-	expression tag	UNP C4XPQ7
C	46	PHE	TYR	conflict	UNP C4XPQ7
C	65	PHE	TYR	conflict	UNP C4XPQ7
C	68	LEU	GLU	conflict	UNP C4XPQ7
C	124	ILE	MET	conflict	UNP C4XPQ7
C	140	ALA	GLU	conflict	UNP C4XPQ7
C	141	ALA	LYS	conflict	UNP C4XPQ7
C	143	ALA	GLU	conflict	UNP C4XPQ7
C	218	GLU	-	expression tag	UNP C4XPQ7
C	219	LEU	-	expression tag	UNP C4XPQ7
C	220	ALA	-	expression tag	UNP C4XPQ7
C	221	LEU	-	expression tag	UNP C4XPQ7
C	222	VAL	-	expression tag	UNP C4XPQ7
C	223	PRO	-	expression tag	UNP C4XPQ7
C	224	ARG	-	expression tag	UNP C4XPQ7
C	225	GLY	-	expression tag	UNP C4XPQ7
C	226	SER	-	expression tag	UNP C4XPQ7
C	227	SER	-	expression tag	UNP C4XPQ7
C	228	ALA	-	expression tag	UNP C4XPQ7
C	229	HIS	-	expression tag	UNP C4XPQ7
C	230	HIS	-	expression tag	UNP C4XPQ7
C	231	HIS	-	expression tag	UNP C4XPQ7
C	232	HIS	-	expression tag	UNP C4XPQ7
C	233	HIS	-	expression tag	UNP C4XPQ7
C	234	HIS	-	expression tag	UNP C4XPQ7
C	235	HIS	-	expression tag	UNP C4XPQ7
C	236	HIS	-	expression tag	UNP C4XPQ7
C	237	HIS	-	expression tag	UNP C4XPQ7
C	238	HIS	-	expression tag	UNP C4XPQ7
D	37	MET	-	initiating methionine	UNP C4XPQ7
D	38	ALA	-	expression tag	UNP C4XPQ7
D	39	MET	-	expression tag	UNP C4XPQ7
D	40	GLY	-	expression tag	UNP C4XPQ7
D	46	PHE	TYR	conflict	UNP C4XPQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	65	PHE	TYR	conflict	UNP C4XPQ7
D	68	LEU	GLU	conflict	UNP C4XPQ7
D	124	ILE	MET	conflict	UNP C4XPQ7
D	140	ALA	GLU	conflict	UNP C4XPQ7
D	141	ALA	LYS	conflict	UNP C4XPQ7
D	143	ALA	GLU	conflict	UNP C4XPQ7
D	218	GLU	-	expression tag	UNP C4XPQ7
D	219	LEU	-	expression tag	UNP C4XPQ7
D	220	ALA	-	expression tag	UNP C4XPQ7
D	221	LEU	-	expression tag	UNP C4XPQ7
D	222	VAL	-	expression tag	UNP C4XPQ7
D	223	PRO	-	expression tag	UNP C4XPQ7
D	224	ARG	-	expression tag	UNP C4XPQ7
D	225	GLY	-	expression tag	UNP C4XPQ7
D	226	SER	-	expression tag	UNP C4XPQ7
D	227	SER	-	expression tag	UNP C4XPQ7
D	228	ALA	-	expression tag	UNP C4XPQ7
D	229	HIS	-	expression tag	UNP C4XPQ7
D	230	HIS	-	expression tag	UNP C4XPQ7
D	231	HIS	-	expression tag	UNP C4XPQ7
D	232	HIS	-	expression tag	UNP C4XPQ7
D	233	HIS	-	expression tag	UNP C4XPQ7
D	234	HIS	-	expression tag	UNP C4XPQ7
D	235	HIS	-	expression tag	UNP C4XPQ7
D	236	HIS	-	expression tag	UNP C4XPQ7
D	237	HIS	-	expression tag	UNP C4XPQ7
D	238	HIS	-	expression tag	UNP C4XPQ7
E	37	MET	-	initiating methionine	UNP C4XPQ7
E	38	ALA	-	expression tag	UNP C4XPQ7
E	39	MET	-	expression tag	UNP C4XPQ7
E	40	GLY	-	expression tag	UNP C4XPQ7
E	46	PHE	TYR	conflict	UNP C4XPQ7
E	65	PHE	TYR	conflict	UNP C4XPQ7
E	68	LEU	GLU	conflict	UNP C4XPQ7
E	124	ILE	MET	conflict	UNP C4XPQ7
E	140	ALA	GLU	conflict	UNP C4XPQ7
E	141	ALA	LYS	conflict	UNP C4XPQ7
E	143	ALA	GLU	conflict	UNP C4XPQ7
E	218	GLU	-	expression tag	UNP C4XPQ7
E	219	LEU	-	expression tag	UNP C4XPQ7
E	220	ALA	-	expression tag	UNP C4XPQ7
E	221	LEU	-	expression tag	UNP C4XPQ7

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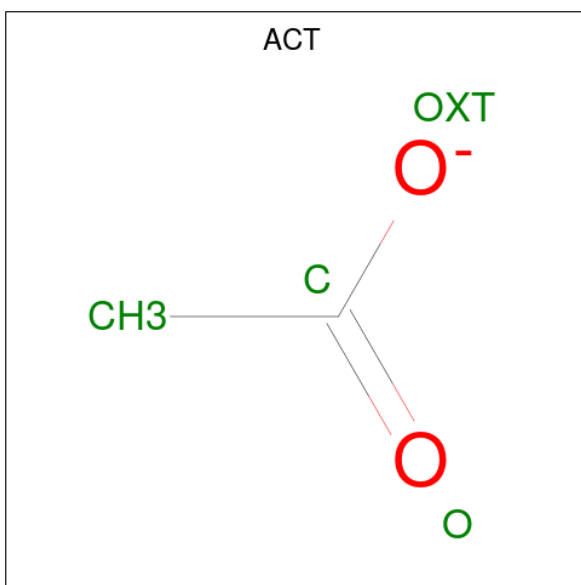
Chain	Residue	Modelled	Actual	Comment	Reference
E	222	VAL	-	expression tag	UNP C4XPQ7
E	223	PRO	-	expression tag	UNP C4XPQ7
E	224	ARG	-	expression tag	UNP C4XPQ7
E	225	GLY	-	expression tag	UNP C4XPQ7
E	226	SER	-	expression tag	UNP C4XPQ7
E	227	SER	-	expression tag	UNP C4XPQ7
E	228	ALA	-	expression tag	UNP C4XPQ7
E	229	HIS	-	expression tag	UNP C4XPQ7
E	230	HIS	-	expression tag	UNP C4XPQ7
E	231	HIS	-	expression tag	UNP C4XPQ7
E	232	HIS	-	expression tag	UNP C4XPQ7
E	233	HIS	-	expression tag	UNP C4XPQ7
E	234	HIS	-	expression tag	UNP C4XPQ7
E	235	HIS	-	expression tag	UNP C4XPQ7
E	236	HIS	-	expression tag	UNP C4XPQ7
E	237	HIS	-	expression tag	UNP C4XPQ7
E	238	HIS	-	expression tag	UNP C4XPQ7
F	37	MET	-	initiating methionine	UNP C4XPQ7
F	38	ALA	-	expression tag	UNP C4XPQ7
F	39	MET	-	expression tag	UNP C4XPQ7
F	40	GLY	-	expression tag	UNP C4XPQ7
F	46	PHE	TYR	conflict	UNP C4XPQ7
F	65	PHE	TYR	conflict	UNP C4XPQ7
F	68	LEU	GLU	conflict	UNP C4XPQ7
F	124	ILE	MET	conflict	UNP C4XPQ7
F	140	ALA	GLU	conflict	UNP C4XPQ7
F	141	ALA	LYS	conflict	UNP C4XPQ7
F	143	ALA	GLU	conflict	UNP C4XPQ7
F	218	GLU	-	expression tag	UNP C4XPQ7
F	219	LEU	-	expression tag	UNP C4XPQ7
F	220	ALA	-	expression tag	UNP C4XPQ7
F	221	LEU	-	expression tag	UNP C4XPQ7
F	222	VAL	-	expression tag	UNP C4XPQ7
F	223	PRO	-	expression tag	UNP C4XPQ7
F	224	ARG	-	expression tag	UNP C4XPQ7
F	225	GLY	-	expression tag	UNP C4XPQ7
F	226	SER	-	expression tag	UNP C4XPQ7
F	227	SER	-	expression tag	UNP C4XPQ7
F	228	ALA	-	expression tag	UNP C4XPQ7
F	229	HIS	-	expression tag	UNP C4XPQ7
F	230	HIS	-	expression tag	UNP C4XPQ7
F	231	HIS	-	expression tag	UNP C4XPQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	232	HIS	-	expression tag	UNP C4XPQ7
F	233	HIS	-	expression tag	UNP C4XPQ7
F	234	HIS	-	expression tag	UNP C4XPQ7
F	235	HIS	-	expression tag	UNP C4XPQ7
F	236	HIS	-	expression tag	UNP C4XPQ7
F	237	HIS	-	expression tag	UNP C4XPQ7
F	238	HIS	-	expression tag	UNP C4XPQ7

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is water.

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.12Å 150.12Å 203.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	120.90 – 3.28 120.90 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (120.90-3.28) 99.9 (120.90-3.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 3.25Å)	Xtrriage
Refinement program	REFMAC 5.8.0151	Depositor
R, $R_{free}$	0.171 , 0.188 0.175 , 0.191	Depositor DCC
$R_{free}$ test set	1740 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	91.3	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.008 for $-1/2^*h+1/2^*k-1/2^*l, 1/2^*h-1/2^*k-1/2^*l, -h-k$ 0.000 for $-1/2^*h+1/2^*k+1/2^*l, 1/2^*h-1/2^*k+1/2^*l, h+k$ 0.000 for $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$ 0.005 for $-1/2^*h-1/2^*k-1/2^*l, -1/2^*h-1/2^*k+1/2^*l, -h+k$ 0.024 for $-h, k, -l$	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8563	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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: ACT, CL

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	0.66	0/1451	0.97	0/1951
1	B	0.66	0/1445	0.98	0/1943
1	C	0.63	0/1445	0.97	0/1943
1	D	0.64	0/1445	0.94	0/1943
1	E	0.66	0/1451	0.99	2/1951 (0.1%)
1	F	0.68	1/1459 (0.1%)	0.96	0/1962
All	All	0.65	1/8696 (0.0%)	0.97	2/11693 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	213	ASP	CA-C	6.27	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	56	ARG	CA-C-N	6.61	134.37	121.41
1	E	56	ARG	C-N-CA	6.61	134.37	121.41

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	56	ARG	Peptide
1	E	57	GLY	Mainchain

## 5.2 Too-close contacts [i](#)

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	1423	0	1439	19	0
1	B	1417	0	1434	18	0
1	C	1417	0	1434	20	0
1	D	1417	0	1434	13	0
1	E	1423	0	1439	20	0
1	F	1431	0	1443	25	0
2	A	4	0	3	0	0
2	B	4	0	3	1	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	F	4	0	3	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	8563	0	8641	111	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 6.

The worst 5 of 111 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:202:PHE:O	1:E:205:VAL:HG12	1.72	0.88
1:F:127:TYR:O	1:F:131:LEU:HD12	1.83	0.78
1:E:187:PHE:O	1:E:190:VAL:HG22	1.87	0.74
1:A:187:PHE:O	1:A:190:VAL:HG22	1.87	0.74
1:C:127:TYR:O	1:C:131:LEU:HD22	1.90	0.72

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	175/202 (87%)	168 (96%)	7 (4%)	0	100	100
1	B	174/202 (86%)	168 (97%)	6 (3%)	0	100	100
1	C	174/202 (86%)	168 (97%)	6 (3%)	0	100	100
1	D	174/202 (86%)	168 (97%)	6 (3%)	0	100	100
1	E	175/202 (87%)	167 (95%)	8 (5%)	0	100	100
1	F	176/202 (87%)	169 (96%)	7 (4%)	0	100	100
All	All	1048/1212 (86%)	1008 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	146/168 (87%)	132 (90%)	14 (10%)	8	29
1	B	145/168 (86%)	133 (92%)	12 (8%)	10	35
1	C	145/168 (86%)	129 (89%)	16 (11%)	6	23
1	D	145/168 (86%)	132 (91%)	13 (9%)	9	31
1	E	146/168 (87%)	136 (93%)	10 (7%)	14	42
1	F	147/168 (88%)	133 (90%)	14 (10%)	8	29
All	All	874/1008 (87%)	795 (91%)	79 (9%)	9	31

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	90	LEU
1	F	124	ILE
1	E	120	VAL
1	F	48	ASN
1	F	179	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	189	ASN
1	F	126	GLN
1	F	189	ASN
1	F	89	ASN
1	C	189	ASN

### 5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
2	ACT	E	301	-	3,3,3	0.77	0	3,3,3	0.93	0
2	ACT	B	301	-	3,3,3	0.78	0	3,3,3	0.83	0
2	ACT	D	301	-	3,3,3	0.77	0	3,3,3	0.89	0
2	ACT	F	301	-	3,3,3	0.88	0	3,3,3	0.50	0
2	ACT	A	301	-	3,3,3	0.76	0	3,3,3	0.97	0
2	ACT	C	301	-	3,3,3	0.87	0	3,3,3	0.70	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	ACT	1	0
2	F	301	ACT	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	177/202 (87%)	-0.46	2 (1%) 78 61	67, 88, 137, 180	1 (0%)
1	B	176/202 (87%)	-0.50	0 100 100	67, 88, 134, 168	0
1	C	176/202 (87%)	-0.46	0 100 100	82, 107, 145, 167	0
1	D	176/202 (87%)	-0.52	0 100 100	74, 97, 133, 163	0
1	E	177/202 (87%)	-0.45	1 (0%) 85 72	84, 105, 140, 176	0
1	F	178/202 (88%)	-0.48	0 100 100	79, 98, 148, 200	0
All	All	1060/1212 (87%)	-0.48	3 (0%) 90 82	67, 100, 140, 200	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	GLN	3.1
1	A	214	SER	2.2
1	E	38	ALA	2.2

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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
2	ACT	C	301	4/4	0.74	0.31	113,121,125,127	0
3	CL	E	302	1/1	0.93	0.13	122,122,122,122	0
3	CL	C	303	1/1	0.94	0.10	106,106,106,106	0
2	ACT	A	301	4/4	0.95	0.16	104,111,113,115	0
3	CL	D	302	1/1	0.95	0.11	108,108,108,108	0
2	ACT	E	301	4/4	0.95	0.15	119,130,134,137	0
3	CL	B	302	1/1	0.96	0.11	112,112,112,112	0
2	ACT	D	301	4/4	0.96	0.11	104,117,121,122	0
3	CL	C	302	1/1	0.97	0.11	117,117,117,117	0
2	ACT	F	301	4/4	0.97	0.15	108,118,125,126	0
3	CL	A	302	1/1	0.97	0.08	105,105,105,105	0
2	ACT	B	301	4/4	0.97	0.14	100,112,116,117	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.