



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 04:57 AM UTC

PDB ID : 5LFL / pdb\_000051fl  
Title : MamA RS-1 Ars<sup>TM</sup> double mutant  
Authors : Zarivach, R.; Cronin, S.L.  
Deposited on : 2016-07-03  
Resolution : 3.37 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  
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

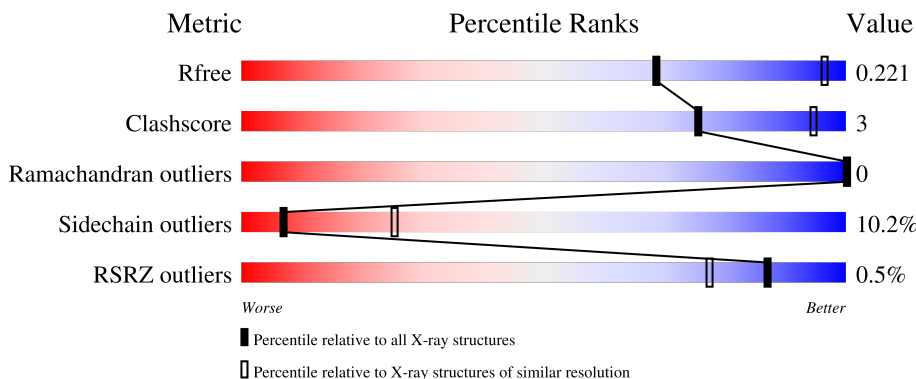
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.37 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	 76% 10% 12%
1	B	202	 74% 11% 13%
1	C	202	 75% 11% 13%
1	D	202	 74% 12% 13%
1	E	202	 74% 12% 12%

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Mol	Chain	Length	Quality of chain
1	F	202	 77% 10% 12%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8547 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	1424	904	255	258	7	0	0	0
1	B	175	1418	902	256	253	7	0	1	0
1	C	175	1417	902	255	253	7	0	1	0
1	D	176	1418	901	254	256	7	0	0	0
1	E	177	1424	904	255	258	7	0	0	0
1	F	178	1432	908	256	261	7	0	0	0

There are 186 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	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
A	224	ARG	-	expression tag	UNP C4XPQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
B	234	HIS	-	expression tag	UNP C4XPQ7
B	235	HIS	-	expression tag	UNP C4XPQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
D	65	PHE	TYR	conflict	UNP C4XPQ7
D	124	ILE	MET	conflict	UNP C4XPQ7
D	140	ALA	GLU	conflict	UNP C4XPQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	238	HIS	-	expression tag	UNP C4XPQ7

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	3	Total O 3 3	0	0
3	D	1	Total O 1 1	0	0
3	E	1	Total O 1 1	0	0
3	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, $\alpha$ , $\beta$ , $\gamma$	150.55Å 150.55Å 204.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 3.37 47.92 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.92-3.37) 99.5 (47.92-3.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.23 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0151	Depositor
R, $R_{free}$	0.196 , 0.214 0.202 , 0.221	Depositor DCC
$R_{free}$ test set	1620 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.5	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 20.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.005 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 $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$ 0.000 for $-1/2^*h-1/2^*k-1/2^*l, -1/2^*h-1/2^*k+1/2^*l, -h+k$ 0.016 for $-h, k, -l$	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% 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: 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	0.78	0/1452	1.03	2/1952 (0.1%)
1	B	0.77	0/1449	1.02	1/1948 (0.1%)
1	C	0.76	0/1449	1.00	0/1948
1	D	0.75	1/1446 (0.1%)	1.00	1/1944 (0.1%)
1	E	0.75	0/1452	1.03	2/1952 (0.1%)
1	F	0.76	0/1460	1.01	0/1963
All	All	0.76	1/8708 (0.0%)	1.01	6/11707 (0.1%)

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	C	0	1
1	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	211	SER	CA-C	5.50	1.60	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	213	ASP	N-CA-C	9.19	122.16	109.11
1	E	71	ARG	CB-CG-CD	5.45	123.84	111.30
1	B	162	GLU	CA-CB-CG	5.38	124.86	114.10
1	A	162	GLU	CA-CB-CG	5.36	124.82	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	MET	N-CA-C	5.01	117.47	111.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	211	SER	Peptide
1	F	214	SER	Peptide

## 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	1424	0	1434	7	0
1	B	1418	0	1438	11	0
1	C	1417	0	1432	9	0
1	D	1418	0	1429	10	0
1	E	1424	0	1434	10	0
1	F	1432	0	1438	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	8547	0	8605	52	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 3.

The worst 5 of 52 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:134:LEU:HA	1:E:137:VAL:HG13	1.74	0.69
1:B:138:VAL:HG13	1:B:148:TYR:CZ	2.38	0.58
1:D:138:VAL:CG1	1:D:148:TYR:CZ	2.88	0.57
1:E:138:VAL:CG1	1:E:148:TYR:CZ	2.88	0.56
1:C:138:VAL:CG1	1:C:148:TYR:CZ	2.88	0.56

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%)	172 (98%)	3 (2%)	0	100	100
1	B	174/202 (86%)	170 (98%)	4 (2%)	0	100	100
1	C	174/202 (86%)	170 (98%)	4 (2%)	0	100	100
1	D	174/202 (86%)	169 (97%)	5 (3%)	0	100	100
1	E	175/202 (87%)	171 (98%)	4 (2%)	0	100	100
1	F	176/202 (87%)	172 (98%)	4 (2%)	0	100	100
All	All	1048/1212 (86%)	1024 (98%)	24 (2%)	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%)	131 (90%)	15 (10%)	7	25
1	B	145/168 (86%)	128 (88%)	17 (12%)	5	20
1	C	145/168 (86%)	133 (92%)	12 (8%)	10	35
1	D	145/168 (86%)	130 (90%)	15 (10%)	7	25
1	E	146/168 (87%)	131 (90%)	15 (10%)	7	25
1	F	147/168 (88%)	132 (90%)	15 (10%)	7	25
All	All	874/1008 (87%)	785 (90%)	89 (10%)	7	25

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	208	LEU
1	E	196	LYS
1	E	42	LYS
1	E	126	GLN
1	F	94	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	183	GLN
1	E	89	ASN
1	E	51	GLN
1	E	195	HIS
1	B	126	GLN

### 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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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%)	-0.27	2 (1%) 78 64	41, 56, 90, 124	1 (0%)
1	B	175/202 (86%)	-0.25	1 (0%) 85 74	30, 58, 90, 123	2 (1%)
1	C	175/202 (86%)	-0.40	0 100 100	48, 65, 86, 103	1 (0%)
1	D	176/202 (87%)	-0.31	1 (0%) 85 74	57, 73, 94, 115	0
1	E	177/202 (87%)	-0.41	1 (0%) 85 74	48, 67, 107, 134	0
1	F	178/202 (88%)	-0.31	0 100 100	57, 72, 97, 124	0
All	All	1058/1212 (87%)	-0.33	5 (0%) 87 77	30, 67, 95, 134	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	GLN	7.0
1	A	212	GLN	4.6
1	A	38	ALA	2.8
1	E	214	SER	2.3
1	D	38	ALA	2.0

### 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	CL	D	400	1/1	0.90	0.08	59,59,59,59	0
2	CL	C	301	1/1	0.94	0.07	59,59,59,59	0
2	CL	C	302	1/1	0.94	0.16	59,59,59,59	0
2	CL	B	400	1/1	0.94	0.10	59,59,59,59	0
2	CL	A	400	1/1	0.95	0.10	59,59,59,59	0
2	CL	E	400	1/1	0.95	0.07	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.