



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:04 AM GMT

PDB ID : 3NO1  
Title : Crystal Structure of Mandelate racemase/muconate lactonizing enzyme from a Marine actinobacterium in complex with magnesium  
Authors : Satyanarayana, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2010-06-24  
Resolution : 2.16 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

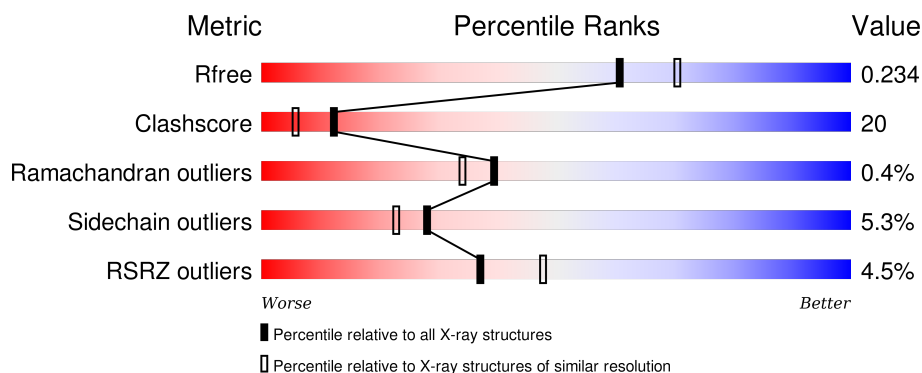
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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. 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	398	<div> <div>2%</div> <div>64% 23% • 11%</div> </div>
1	B	398	<div> <div>6%</div> <div>59% 26% • 12%</div> </div>
1	C	398	<div> <div>•</div> <div>65% 23% • 10%</div> </div>
1	D	398	<div> <div>7%</div> <div>57% 29% • 12%</div> </div>
1	E	398	<div> <div>4%</div> <div>56% 29% • 11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	398	<div><div></div><div>4%</div><div>57%</div><div>28%</div><div>•</div><div>12%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17170 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 Mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	Se	0	0	0
			2782	1757	488	522	5	10			
1	B	349	Total	C	N	O	S	Se	0	0	0
			2734	1726	477	516	5	10			
1	C	357	Total	C	N	O	S	Se	0	0	0
			2792	1762	490	525	5	10			
1	D	350	Total	C	N	O	S	Se	0	0	0
			2745	1732	481	517	5	10			
1	E	353	Total	C	N	O	S	Se	0	0	0
			2762	1742	484	521	5	10			
1	F	349	Total	C	N	O	S	Se	0	0	0
			2723	1718	476	514	5	10			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP A4AFX2
A	0	SER	-	expression tag	UNP A4AFX2
A	1	LEU	-	expression tag	UNP A4AFX2
A	389	GLU	-	expression tag	UNP A4AFX2
A	390	GLY	-	expression tag	UNP A4AFX2
A	391	HIS	-	expression tag	UNP A4AFX2
A	392	HIS	-	expression tag	UNP A4AFX2
A	393	HIS	-	expression tag	UNP A4AFX2
A	394	HIS	-	expression tag	UNP A4AFX2
A	395	HIS	-	expression tag	UNP A4AFX2
A	396	HIS	-	expression tag	UNP A4AFX2
B	-1	MSE	-	expression tag	UNP A4AFX2
B	0	SER	-	expression tag	UNP A4AFX2
B	1	LEU	-	expression tag	UNP A4AFX2
B	389	GLU	-	expression tag	UNP A4AFX2
B	390	GLY	-	expression tag	UNP A4AFX2
B	391	HIS	-	expression tag	UNP A4AFX2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	392	HIS	-	expression tag	UNP A4AFX2
B	393	HIS	-	expression tag	UNP A4AFX2
B	394	HIS	-	expression tag	UNP A4AFX2
B	395	HIS	-	expression tag	UNP A4AFX2
B	396	HIS	-	expression tag	UNP A4AFX2
C	-1	MSE	-	expression tag	UNP A4AFX2
C	0	SER	-	expression tag	UNP A4AFX2
C	1	LEU	-	expression tag	UNP A4AFX2
C	389	GLU	-	expression tag	UNP A4AFX2
C	390	GLY	-	expression tag	UNP A4AFX2
C	391	HIS	-	expression tag	UNP A4AFX2
C	392	HIS	-	expression tag	UNP A4AFX2
C	393	HIS	-	expression tag	UNP A4AFX2
C	394	HIS	-	expression tag	UNP A4AFX2
C	395	HIS	-	expression tag	UNP A4AFX2
C	396	HIS	-	expression tag	UNP A4AFX2
D	-1	MSE	-	expression tag	UNP A4AFX2
D	0	SER	-	expression tag	UNP A4AFX2
D	1	LEU	-	expression tag	UNP A4AFX2
D	389	GLU	-	expression tag	UNP A4AFX2
D	390	GLY	-	expression tag	UNP A4AFX2
D	391	HIS	-	expression tag	UNP A4AFX2
D	392	HIS	-	expression tag	UNP A4AFX2
D	393	HIS	-	expression tag	UNP A4AFX2
D	394	HIS	-	expression tag	UNP A4AFX2
D	395	HIS	-	expression tag	UNP A4AFX2
D	396	HIS	-	expression tag	UNP A4AFX2
E	-1	MSE	-	expression tag	UNP A4AFX2
E	0	SER	-	expression tag	UNP A4AFX2
E	1	LEU	-	expression tag	UNP A4AFX2
E	389	GLU	-	expression tag	UNP A4AFX2
E	390	GLY	-	expression tag	UNP A4AFX2
E	391	HIS	-	expression tag	UNP A4AFX2
E	392	HIS	-	expression tag	UNP A4AFX2
E	393	HIS	-	expression tag	UNP A4AFX2
E	394	HIS	-	expression tag	UNP A4AFX2
E	395	HIS	-	expression tag	UNP A4AFX2
E	396	HIS	-	expression tag	UNP A4AFX2
F	-1	MSE	-	expression tag	UNP A4AFX2
F	0	SER	-	expression tag	UNP A4AFX2
F	1	LEU	-	expression tag	UNP A4AFX2
F	389	GLU	-	expression tag	UNP A4AFX2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	390	GLY	-	expression tag	UNP A4AFX2
F	391	HIS	-	expression tag	UNP A4AFX2
F	392	HIS	-	expression tag	UNP A4AFX2
F	393	HIS	-	expression tag	UNP A4AFX2
F	394	HIS	-	expression tag	UNP A4AFX2
F	395	HIS	-	expression tag	UNP A4AFX2
F	396	HIS	-	expression tag	UNP A4AFX2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

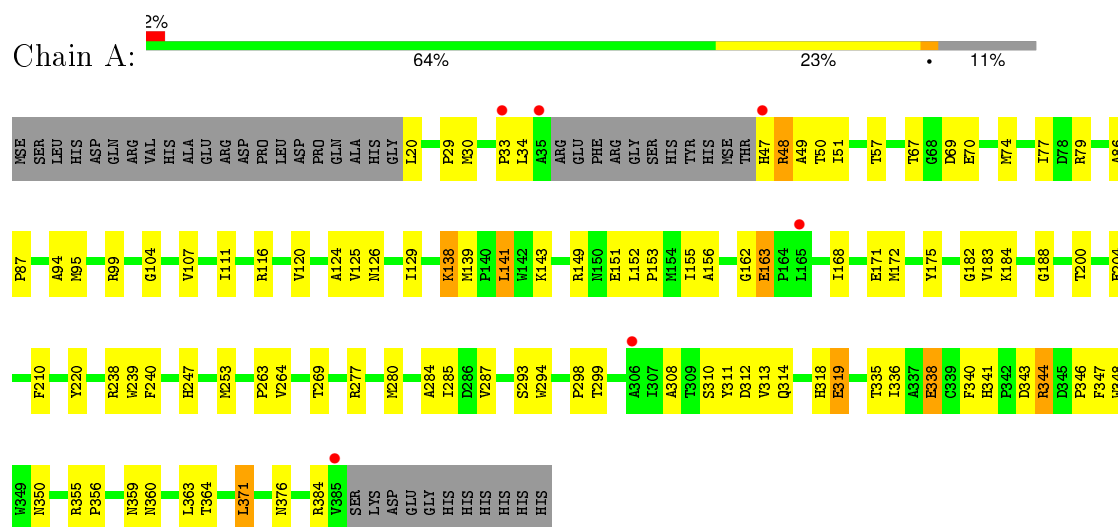
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	137	Total O 137 137	0	0
3	B	84	Total O 84 84	0	0
3	C	136	Total O 136 136	0	0
3	D	88	Total O 88 88	0	0
3	E	80	Total O 80 80	0	0
3	F	101	Total O 101 101	0	0

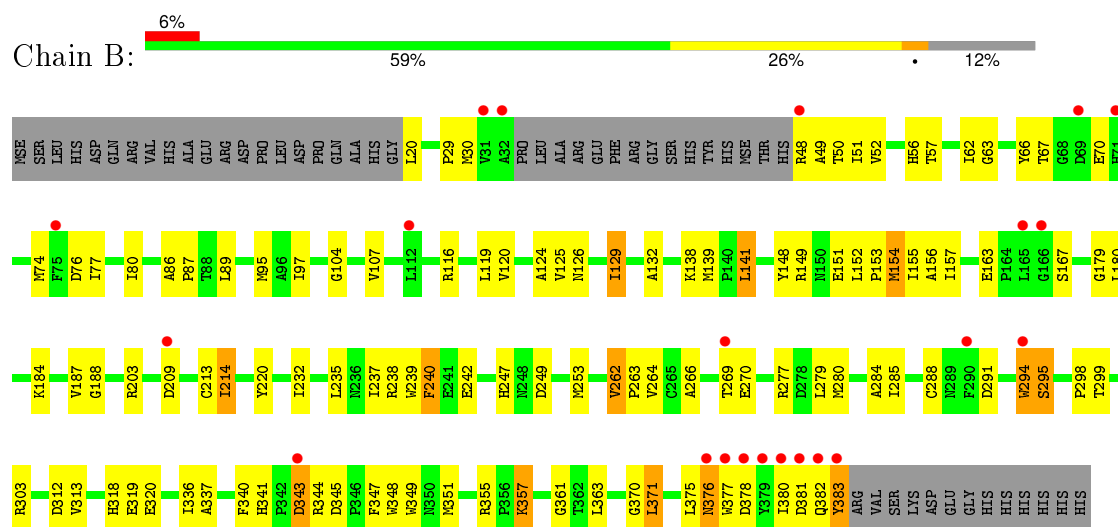
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

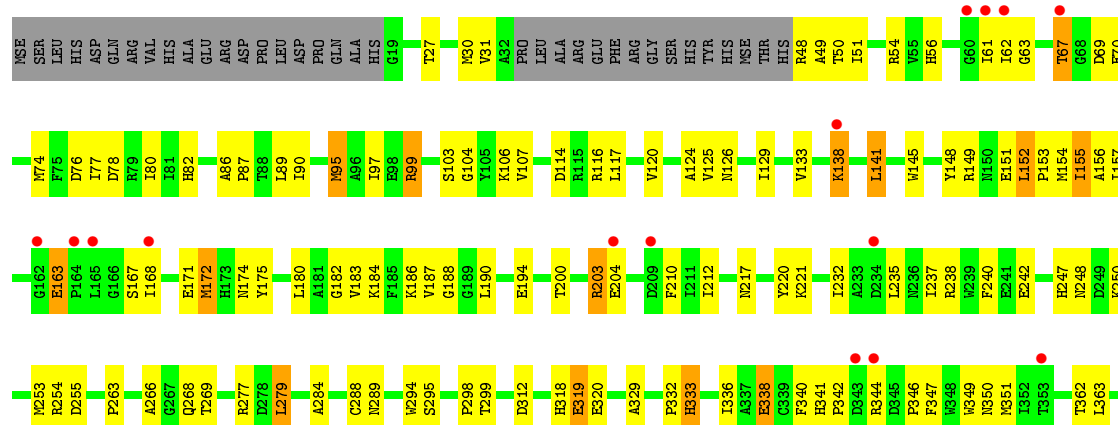


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

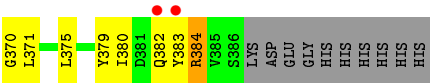


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

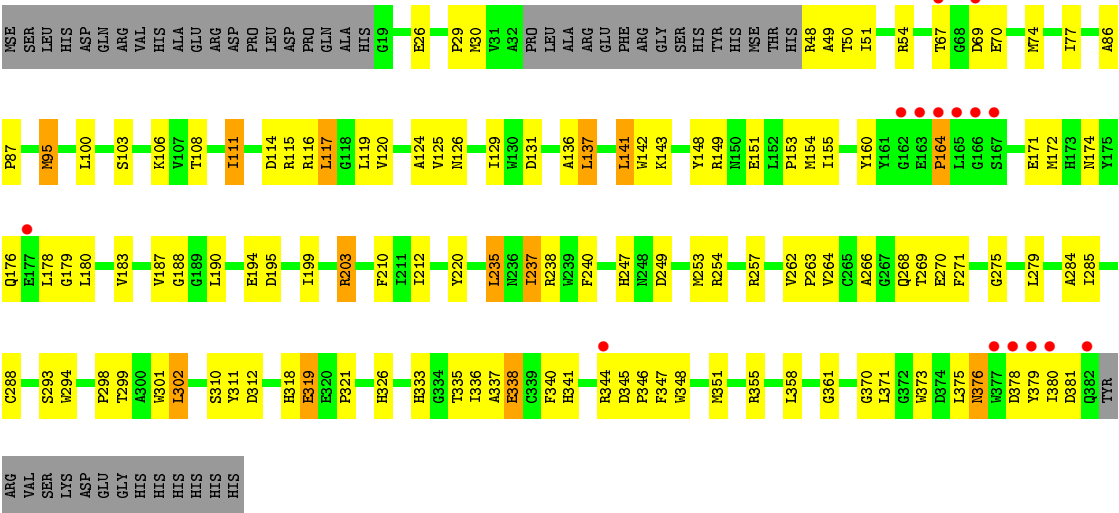








● Molecule 1: Mandelate racemase/muconate lactonizing enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.96Å 90.10Å 94.66Å 115.80° 109.75° 97.58°	Depositor
Resolution (Å)	42.51 – 2.16 42.51 – 2.16	Depositor EDS
% Data completeness (in resolution range)	96.0 (42.51-2.16) 78.5 (42.51-2.16)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.97 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.207 , 0.240 0.202 , 0.234	Depositor DCC
$R_{free}$ test set	4670 reflections (4.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 117788 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG

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	0.33	0/2841	0.63	0/3851
1	B	0.33	0/2791	0.64	0/3782
1	C	0.34	0/2851	0.63	0/3864
1	D	0.33	0/2802	0.63	0/3796
1	E	0.32	0/2819	0.62	0/3819
1	F	0.36	0/2779	0.65	0/3765
All	All	0.34	0/16883	0.63	0/22877

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2782	0	2685	108	0
1	B	2734	0	2632	127	0
1	C	2792	0	2692	84	0
1	D	2745	0	2645	106	0
1	E	2762	0	2662	129	0
1	F	2723	0	2622	113	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	137	0	0	5	0
3	B	84	0	0	8	0
3	C	136	0	0	5	0
3	D	88	0	0	8	0
3	E	80	0	0	4	0
3	F	101	0	0	3	0
All	All	17170	0	15938	640	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 20.

The worst 5 of 640 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:A:253:MSE:HE3	1:A:264:VAL:HG12	1.32	1.07
1:F:30:MSE:HE1	1:F:380:ILE:HG23	1.34	1.05
1:A:253:MSE:HE3	1:A:264:VAL:CG1	1.86	1.05
1:A:280:MSE:HE2	1:A:311:TYR:HB2	1.40	1.04
1:F:253:MSE:HE3	1:F:264:VAL:CG1	1.90	1.01

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	351/398 (88%)	340 (97%)	10 (3%)	1 (0%)	46 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	345/398 (87%)	328 (95%)	16 (5%)	1 (0%)	46	42
1	C	353/398 (89%)	344 (98%)	8 (2%)	1 (0%)	46	42
1	D	346/398 (87%)	331 (96%)	14 (4%)	1 (0%)	46	42
1	E	349/398 (88%)	333 (95%)	14 (4%)	2 (1%)	30	21
1	F	345/398 (87%)	325 (94%)	18 (5%)	2 (1%)	30	21
All	All	2089/2388 (88%)	2001 (96%)	80 (4%)	8 (0%)	39	34

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	319	GLU
1	A	319	GLU
1	F	319	GLU
1	B	187	VAL
1	C	319	GLU

### 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	287/313 (92%)	275 (96%)	12 (4%)	36	34
1	B	282/313 (90%)	265 (94%)	17 (6%)	24	18
1	C	288/313 (92%)	277 (96%)	11 (4%)	40	37
1	D	283/313 (90%)	269 (95%)	14 (5%)	31	26
1	E	285/313 (91%)	265 (93%)	20 (7%)	19	12
1	F	280/313 (90%)	264 (94%)	16 (6%)	25	19
All	All	1705/1878 (91%)	1615 (95%)	90 (5%)	28	23

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	138	LYS

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Mol	Chain	Res	Type
1	D	295	SER
1	F	262	VAL
1	D	141	LEU
1	D	194	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	359	ASN
1	D	247	HIS
1	F	248	ASN
1	C	360	ASN
1	C	382	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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 ⓘ

### 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	345/398 (86%)	-0.10	6 (1%) 73 80	7, 16, 31, 41	0
1	B	339/398 (85%)	0.29	22 (6%) 22 31	8, 21, 38, 43	0
1	C	347/398 (87%)	-0.12	5 (1%) 78 83	7, 16, 31, 40	0
1	D	340/398 (85%)	0.34	28 (8%) 14 20	8, 21, 37, 44	0
1	E	343/398 (86%)	0.24	17 (4%) 32 43	10, 22, 37, 43	0
1	F	339/398 (85%)	0.26	15 (4%) 38 49	7, 22, 38, 48	0
All	All	2053/2388 (85%)	0.15	93 (4%) 37 48	7, 20, 36, 48	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	163	GLU	5.9
1	D	164	PRO	5.9
1	F	165	LEU	5.2
1	D	31	VAL	5.0
1	F	162	GLY	4.9

### 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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	F	397	1/1	0.94	0.13	0.44	26,26,26,26	0
2	MG	B	397	1/1	0.96	0.07	-1.99	25,25,25,25	0
2	MG	C	397	1/1	0.96	0.06	-2.03	16,16,16,16	0
2	MG	A	397	1/1	0.92	0.05	-2.62	19,19,19,19	0
2	MG	E	397	1/1	0.93	0.04	-2.69	29,29,29,29	0
2	MG	D	397	1/1	0.93	0.06	-3.87	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.