



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:45 AM GMT

PDB ID : 3FV9  
Title : Crystal structure of putative mandelate racemase/muconatelactonizing enzyme from ROSEOVARIUS NUBINHIBENS ISM complexed with magnesium  
Authors : Malashkevich, V.N.; Rutter, M.; Bain, K.T.; Lau, C.; Ozyurt, S.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2009-01-15  
Resolution : 1.90 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

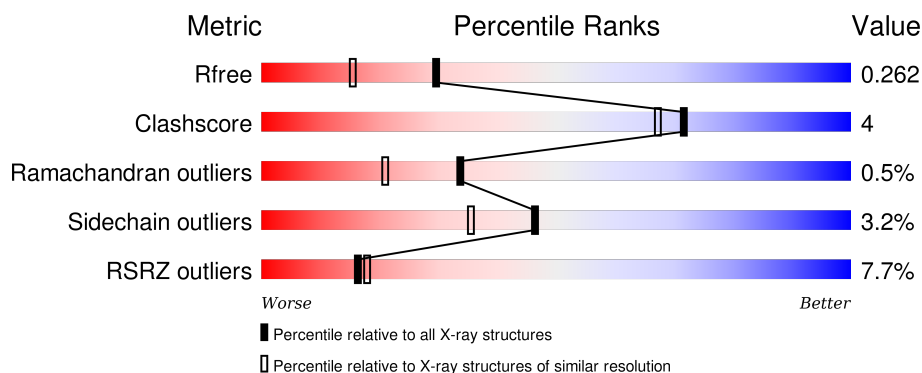
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	386	<div> <div>4%</div> <div>83% 10% • 6%</div> </div>
1	B	386	<div> <div>4%</div> <div>85% 9% • 5%</div> </div>
1	C	386	<div> <div>10%</div> <div>87% 10% • •</div> </div>
1	D	386	<div> <div>5%</div> <div>88% 9% •</div> </div>
1	E	386	<div> <div>9%</div> <div>85% 11% • •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	386	<div><div></div><div>10%</div><div>85%</div><div>11%</div><div></div><div></div></div>
1	G	386	<div><div></div><div>%</div><div>88%</div><div>8%</div><div></div><div></div></div>
1	H	386	<div><div></div><div>17%</div><div>84%</div><div>12%</div><div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24665 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	G	373	Total	C	N	O	S	0	4	0
			2800	1743	515	526	16			
1	A	363	Total	C	N	O	S	0	0	0
			2687	1667	494	510	16			
1	D	373	Total	C	N	O	S	0	0	0
			2767	1718	510	523	16			
1	E	373	Total	C	N	O	S	0	0	0
			2767	1718	510	523	16			
1	F	373	Total	C	N	O	S	0	0	0
			2767	1718	510	523	16			
1	B	365	Total	C	N	O	S	0	0	0
			2704	1679	496	513	16			
1	H	374	Total	C	N	O	S	0	2	0
			2786	1730	513	527	16			
1	C	374	Total	C	N	O	S	0	1	0
			2782	1727	513	526	16			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	MET	-	EXPRESSION TAG	UNP A3SNG0
G	0	SER	-	EXPRESSION TAG	UNP A3SNG0
G	1	LEU	-	EXPRESSION TAG	UNP A3SNG0
G	377	GLU	-	EXPRESSION TAG	UNP A3SNG0
G	378	GLY	-	EXPRESSION TAG	UNP A3SNG0
G	379	HIS	-	EXPRESSION TAG	UNP A3SNG0
G	380	HIS	-	EXPRESSION TAG	UNP A3SNG0
G	381	HIS	-	EXPRESSION TAG	UNP A3SNG0
G	382	HIS	-	EXPRESSION TAG	UNP A3SNG0
G	383	HIS	-	EXPRESSION TAG	UNP A3SNG0
G	384	HIS	-	EXPRESSION TAG	UNP A3SNG0
A	-1	MET	-	EXPRESSION TAG	UNP A3SNG0
A	0	SER	-	EXPRESSION TAG	UNP A3SNG0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	-	EXPRESSION TAG	UNP A3SNG0
A	377	GLU	-	EXPRESSION TAG	UNP A3SNG0
A	378	GLY	-	EXPRESSION TAG	UNP A3SNG0
A	379	HIS	-	EXPRESSION TAG	UNP A3SNG0
A	380	HIS	-	EXPRESSION TAG	UNP A3SNG0
A	381	HIS	-	EXPRESSION TAG	UNP A3SNG0
A	382	HIS	-	EXPRESSION TAG	UNP A3SNG0
A	383	HIS	-	EXPRESSION TAG	UNP A3SNG0
A	384	HIS	-	EXPRESSION TAG	UNP A3SNG0
D	-1	MET	-	EXPRESSION TAG	UNP A3SNG0
D	0	SER	-	EXPRESSION TAG	UNP A3SNG0
D	1	LEU	-	EXPRESSION TAG	UNP A3SNG0
D	377	GLU	-	EXPRESSION TAG	UNP A3SNG0
D	378	GLY	-	EXPRESSION TAG	UNP A3SNG0
D	379	HIS	-	EXPRESSION TAG	UNP A3SNG0
D	380	HIS	-	EXPRESSION TAG	UNP A3SNG0
D	381	HIS	-	EXPRESSION TAG	UNP A3SNG0
D	382	HIS	-	EXPRESSION TAG	UNP A3SNG0
D	383	HIS	-	EXPRESSION TAG	UNP A3SNG0
D	384	HIS	-	EXPRESSION TAG	UNP A3SNG0
E	-1	MET	-	EXPRESSION TAG	UNP A3SNG0
E	0	SER	-	EXPRESSION TAG	UNP A3SNG0
E	1	LEU	-	EXPRESSION TAG	UNP A3SNG0
E	377	GLU	-	EXPRESSION TAG	UNP A3SNG0
E	378	GLY	-	EXPRESSION TAG	UNP A3SNG0
E	379	HIS	-	EXPRESSION TAG	UNP A3SNG0
E	380	HIS	-	EXPRESSION TAG	UNP A3SNG0
E	381	HIS	-	EXPRESSION TAG	UNP A3SNG0
E	382	HIS	-	EXPRESSION TAG	UNP A3SNG0
E	383	HIS	-	EXPRESSION TAG	UNP A3SNG0
E	384	HIS	-	EXPRESSION TAG	UNP A3SNG0
F	-1	MET	-	EXPRESSION TAG	UNP A3SNG0
F	0	SER	-	EXPRESSION TAG	UNP A3SNG0
F	1	LEU	-	EXPRESSION TAG	UNP A3SNG0
F	377	GLU	-	EXPRESSION TAG	UNP A3SNG0
F	378	GLY	-	EXPRESSION TAG	UNP A3SNG0
F	379	HIS	-	EXPRESSION TAG	UNP A3SNG0
F	380	HIS	-	EXPRESSION TAG	UNP A3SNG0
F	381	HIS	-	EXPRESSION TAG	UNP A3SNG0
F	382	HIS	-	EXPRESSION TAG	UNP A3SNG0
F	383	HIS	-	EXPRESSION TAG	UNP A3SNG0
F	384	HIS	-	EXPRESSION TAG	UNP A3SNG0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	EXPRESSION TAG	UNP A3SNG0
B	0	SER	-	EXPRESSION TAG	UNP A3SNG0
B	1	LEU	-	EXPRESSION TAG	UNP A3SNG0
B	377	GLU	-	EXPRESSION TAG	UNP A3SNG0
B	378	GLY	-	EXPRESSION TAG	UNP A3SNG0
B	379	HIS	-	EXPRESSION TAG	UNP A3SNG0
B	380	HIS	-	EXPRESSION TAG	UNP A3SNG0
B	381	HIS	-	EXPRESSION TAG	UNP A3SNG0
B	382	HIS	-	EXPRESSION TAG	UNP A3SNG0
B	383	HIS	-	EXPRESSION TAG	UNP A3SNG0
B	384	HIS	-	EXPRESSION TAG	UNP A3SNG0
H	-1	MET	-	EXPRESSION TAG	UNP A3SNG0
H	0	SER	-	EXPRESSION TAG	UNP A3SNG0
H	1	LEU	-	EXPRESSION TAG	UNP A3SNG0
H	377	GLU	-	EXPRESSION TAG	UNP A3SNG0
H	378	GLY	-	EXPRESSION TAG	UNP A3SNG0
H	379	HIS	-	EXPRESSION TAG	UNP A3SNG0
H	380	HIS	-	EXPRESSION TAG	UNP A3SNG0
H	381	HIS	-	EXPRESSION TAG	UNP A3SNG0
H	382	HIS	-	EXPRESSION TAG	UNP A3SNG0
H	383	HIS	-	EXPRESSION TAG	UNP A3SNG0
H	384	HIS	-	EXPRESSION TAG	UNP A3SNG0
C	-1	MET	-	EXPRESSION TAG	UNP A3SNG0
C	0	SER	-	EXPRESSION TAG	UNP A3SNG0
C	1	LEU	-	EXPRESSION TAG	UNP A3SNG0
C	377	GLU	-	EXPRESSION TAG	UNP A3SNG0
C	378	GLY	-	EXPRESSION TAG	UNP A3SNG0
C	379	HIS	-	EXPRESSION TAG	UNP A3SNG0
C	380	HIS	-	EXPRESSION TAG	UNP A3SNG0
C	381	HIS	-	EXPRESSION TAG	UNP A3SNG0
C	382	HIS	-	EXPRESSION TAG	UNP A3SNG0
C	383	HIS	-	EXPRESSION TAG	UNP A3SNG0
C	384	HIS	-	EXPRESSION TAG	UNP A3SNG0

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		

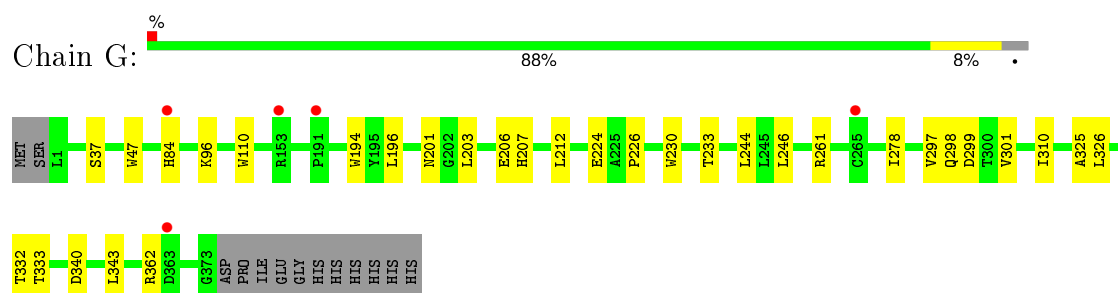
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2600	Total	O	0	0
			2600	2600		

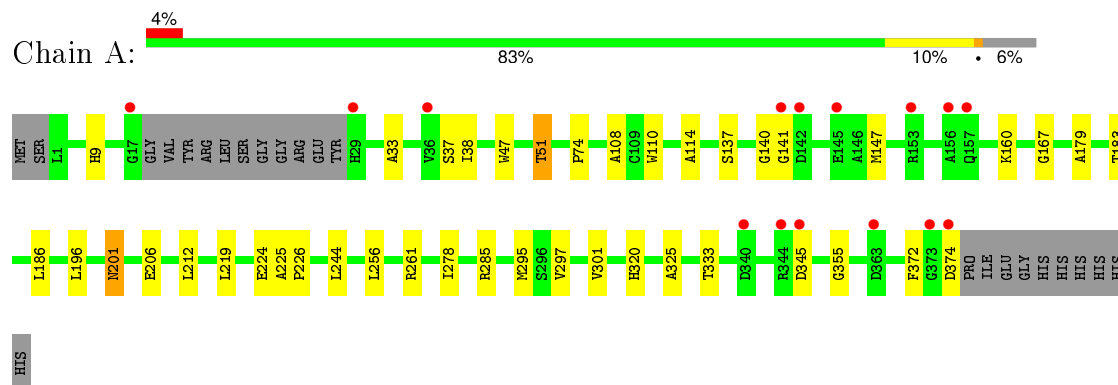
### 3 Residue-property plots

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.

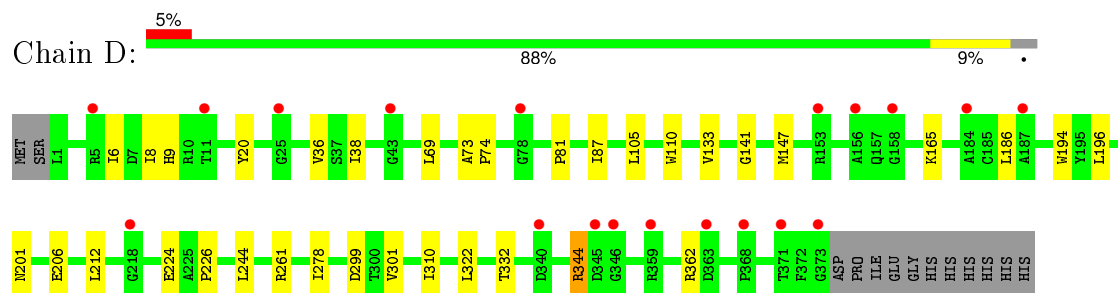
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



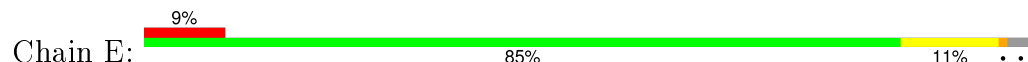
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



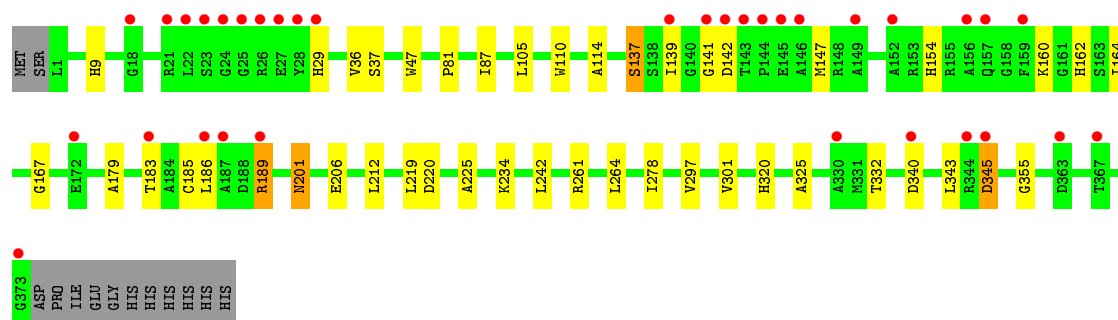
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



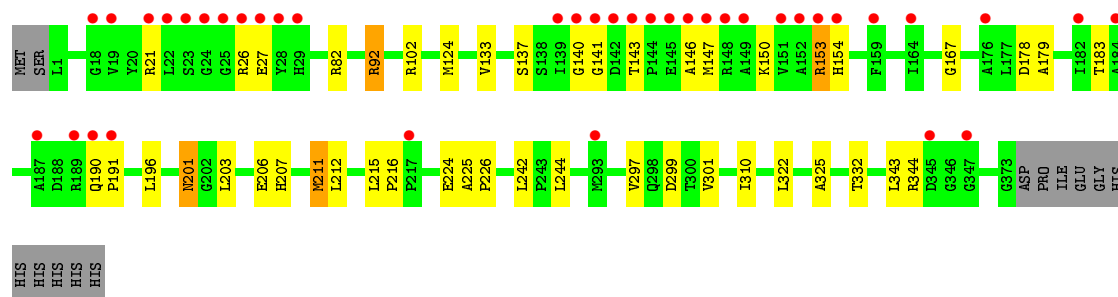
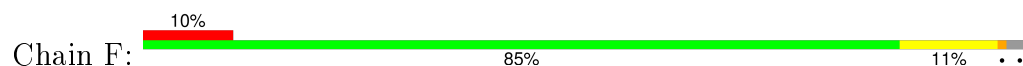
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



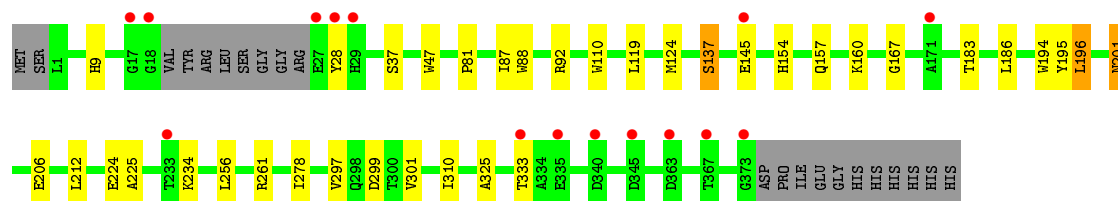
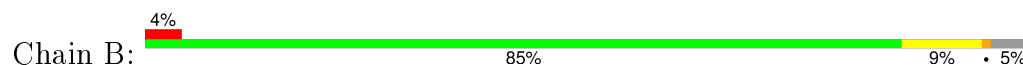




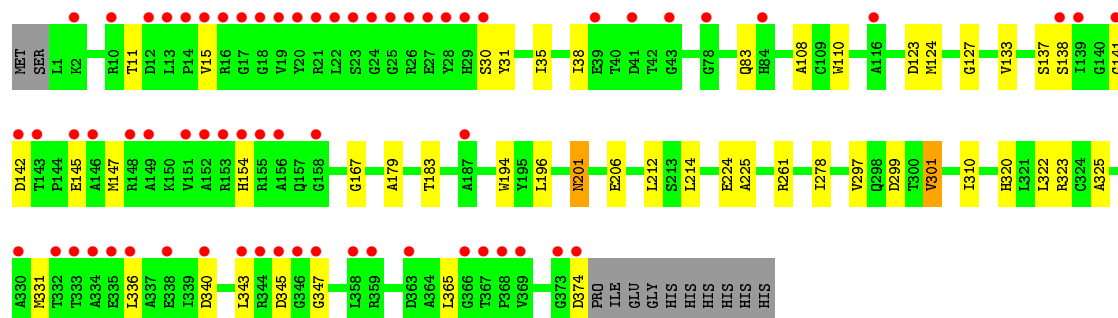
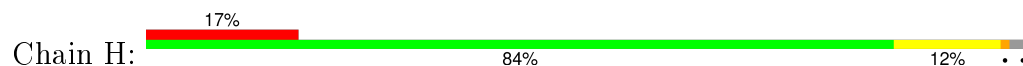
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



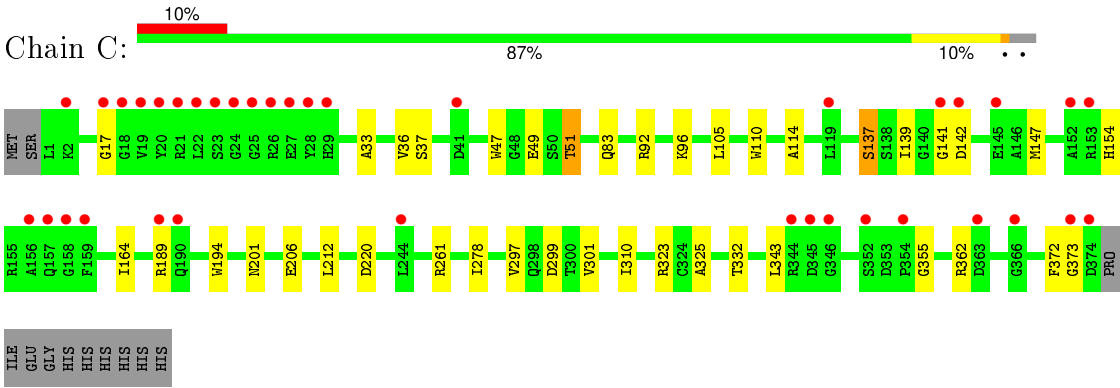
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- 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 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.08Å 174.57Å 108.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-1.90) 95.7 (20.00-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.49 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.203 , 0.241 0.229 , 0.262	Depositor DCC
$R_{free}$ test set	12030 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.0	EDS
Estimated twinning fraction	0.000 for k,h,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	3 of 239779 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24665	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.69% 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	0.43	0/2732	0.59	0/3711
1	B	0.46	0/2750	0.59	1/3735 (0.0%)
1	C	0.45	0/2834	0.61	0/3849
1	D	0.43	0/2815	0.59	0/3823
1	E	0.43	0/2815	0.60	0/3823
1	F	0.51	0/2815	0.63	2/3823 (0.1%)
1	G	0.45	0/2857	0.60	0/3882
1	H	0.42	0/2841	0.59	0/3859
All	All	0.45	0/22459	0.60	3/30505 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	211	MET	CG-SD-CE	6.82	111.11	100.20
1	B	196	LEU	CA-CB-CG	5.37	127.66	115.30
1	F	140	GLY	N-CA-C	5.06	125.74	113.10

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	2687	0	2710	21	0
1	B	2704	0	2724	22	0
1	C	2782	0	2802	23	0
1	D	2767	0	2791	20	0
1	E	2767	0	2791	24	0
1	F	2767	0	2791	33	0
1	G	2800	0	2824	18	0
1	H	2786	0	2809	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	G	2600	0	0	32	0
All	All	24665	0	22242	192	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 4.

The worst 5 of 192 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)
3:G:2043:HOH:O	1:E:340:ASP:HB2	1.58	1.03
1:F:141:GLY:HA2	1:F:147:MET:CE	1.90	1.01
1:F:141:GLY:HA2	1:F:147:MET:HE3	1.40	0.99
1:C:141:GLY:HA2	1:C:147:MET:CE	1.98	0.94
1:F:178:ASP:HB3	1:F:211:MET:HE1	1.48	0.93

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	359/386 (93%)	349 (97%)	8 (2%)	2 (1%)	30	17
1	B	361/386 (94%)	351 (97%)	8 (2%)	2 (1%)	30	17
1	C	373/386 (97%)	363 (97%)	8 (2%)	2 (0%)	34	21
1	D	371/386 (96%)	362 (98%)	8 (2%)	1 (0%)	46	35
1	E	371/386 (96%)	361 (97%)	7 (2%)	3 (1%)	24	11
1	F	371/386 (96%)	358 (96%)	11 (3%)	2 (0%)	34	21
1	G	375/386 (97%)	364 (97%)	10 (3%)	1 (0%)	46	35
1	H	374/386 (97%)	364 (97%)	8 (2%)	2 (0%)	34	21
All	All	2955/3088 (96%)	2872 (97%)	68 (2%)	15 (0%)	34	21

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	GLY
1	A	301	VAL
1	F	301	VAL
1	B	301	VAL
1	C	301	VAL

### 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	275/294 (94%)	266 (97%)	9 (3%)	45	34
1	B	276/294 (94%)	269 (98%)	7 (2%)	55	47
1	C	284/294 (97%)	274 (96%)	10 (4%)	43	31
1	D	282/294 (96%)	275 (98%)	7 (2%)	55	47
1	E	282/294 (96%)	272 (96%)	10 (4%)	43	31
1	F	282/294 (96%)	269 (95%)	13 (5%)	33	21
1	G	286/294 (97%)	279 (98%)	7 (2%)	57	49
1	H	285/294 (97%)	277 (97%)	8 (3%)	51	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2252/2352 (96%)	2181 (97%)	71 (3%)	46 35

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	345	ASP
1	F	201	ASN
1	C	201	ASN
1	F	92	ARG
1	F	150	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	157	GLN
1	F	154	HIS
1	C	9	HIS
1	E	320	HIS
1	F	201	ASN

### 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 5 ligands modelled in this entry, 5 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	363/386 (94%)	0.35	15 (4%) 41 45	9, 16, 25, 41	0
1	B	365/386 (94%)	0.40	15 (4%) 41 45	8, 16, 24, 51	0
1	C	374/386 (96%)	0.68	37 (9%) 9 10	8, 17, 30, 48	0
1	D	373/386 (96%)	0.52	19 (5%) 32 35	9, 16, 25, 29	0
1	E	373/386 (96%)	0.54	34 (9%) 11 13	10, 17, 29, 46	0
1	F	373/386 (96%)	0.68	39 (10%) 8 9	10, 15, 28, 46	0
1	G	373/386 (96%)	0.27	5 (1%) 79 82	9, 15, 25, 33	0
1	H	374/386 (96%)	0.91	66 (17%) 2 2	8, 16, 31, 49	0
All	All	2968/3088 (96%)	0.54	230 (7%) 16 18	8, 16, 27, 51	0

The worst 5 of 230 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	374	ASP	10.5
1	H	19	VAL	9.2
1	B	18	GLY	8.3
1	C	24	GLY	8.1
1	H	25	GLY	7.7

### 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	501	1/1	0.83	0.20	1.35	41,41,41,41	0
2	MG	E	501	1/1	0.91	0.11	-0.51	35,35,35,35	0
2	MG	C	501	1/1	0.94	0.09	-1.18	37,37,37,37	0
2	MG	A	501	1/1	0.95	0.09	-1.20	23,23,23,23	0
2	MG	B	501	1/1	0.95	0.05	-3.16	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.