



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 09:16 AM EDT

PDB ID : 2RDX  
Title : Crystal structure of mandelate racemase/muconate lactonizing enzyme from *Roseovarius nubinhibens* ISM  
Authors : Patskovsky, Y.; Bonanno, J.; Sauder, J.M.; Ozyurt, S.; Gilmore, M.; Lau, C.; Maletic, M.; Gheyi, T.; Wasserman, S.R.; Koss, J.; Gerlt, J.A.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2007-09-25  
Resolution : 2.00 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

<https://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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)

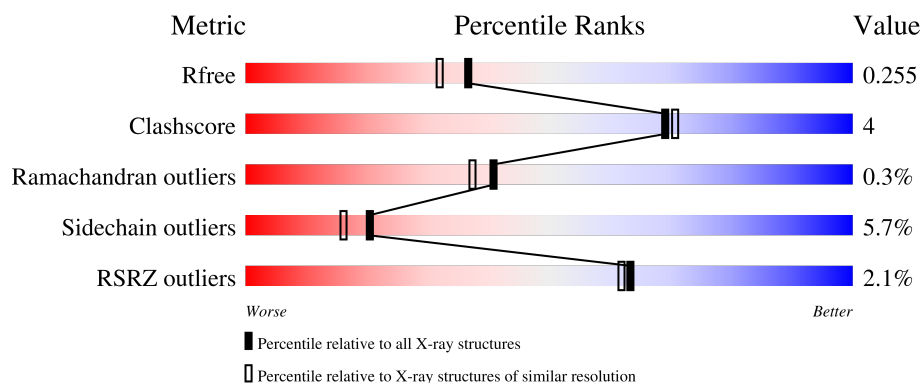
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	379	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	379	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>
1	C	379	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>
1	D	379	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>..</div> </div> </div>

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Validation Pipeline (wwPDB-VP) : 2.36.2

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Mol	Chain	Length	Quality of chain
1	E	379	<div><div></div><div>3%</div><div>85%</div><div>10%</div><div></div><div></div></div>
1	F	379	<div><div></div><div>4%</div><div>87%</div><div>9%</div><div></div><div></div></div>
1	G	379	<div><div></div><div></div><div>85%</div><div>9%</div><div>5%</div><div></div></div>
1	H	379	<div><div></div><div>3%</div><div>89%</div><div>7%</div><div></div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23975 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, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	10	0
			2890	1802	529	538	21			
1	B	369	Total	C	N	O	S	0	4	0
			2851	1776	519	536	20			
1	C	369	Total	C	N	O	S	0	6	0
			2872	1788	531	534	19			
1	D	369	Total	C	N	O	S	0	11	0
			2910	1812	542	537	19			
1	E	369	Total	C	N	O	S	0	6	0
			2865	1786	527	533	19			
1	F	369	Total	C	N	O	S	0	3	0
			2850	1774	522	535	19			
1	G	360	Total	C	N	O	S	0	3	0
			2793	1738	514	522	19			
1	H	369	Total	C	N	O	S	0	6	0
			2869	1788	528	534	19			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP A3SNF8
A	0	SER	-	expression tag	UNP A3SNF8
A	1	LEU	-	expression tag	UNP A3SNF8
A	370	GLU	-	expression tag	UNP A3SNF8
A	371	GLY	-	expression tag	UNP A3SNF8
A	372	HIS	-	expression tag	UNP A3SNF8
A	373	HIS	-	expression tag	UNP A3SNF8
A	374	HIS	-	expression tag	UNP A3SNF8
A	375	HIS	-	expression tag	UNP A3SNF8
A	376	HIS	-	expression tag	UNP A3SNF8
A	377	HIS	-	expression tag	UNP A3SNF8
B	-1	MET	-	expression tag	UNP A3SNF8
B	0	SER	-	expression tag	UNP A3SNF8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	LEU	-	expression tag	UNP A3SNF8
B	370	GLU	-	expression tag	UNP A3SNF8
B	371	GLY	-	expression tag	UNP A3SNF8
B	372	HIS	-	expression tag	UNP A3SNF8
B	373	HIS	-	expression tag	UNP A3SNF8
B	374	HIS	-	expression tag	UNP A3SNF8
B	375	HIS	-	expression tag	UNP A3SNF8
B	376	HIS	-	expression tag	UNP A3SNF8
B	377	HIS	-	expression tag	UNP A3SNF8
C	-1	MET	-	expression tag	UNP A3SNF8
C	0	SER	-	expression tag	UNP A3SNF8
C	1	LEU	-	expression tag	UNP A3SNF8
C	370	GLU	-	expression tag	UNP A3SNF8
C	371	GLY	-	expression tag	UNP A3SNF8
C	372	HIS	-	expression tag	UNP A3SNF8
C	373	HIS	-	expression tag	UNP A3SNF8
C	374	HIS	-	expression tag	UNP A3SNF8
C	375	HIS	-	expression tag	UNP A3SNF8
C	376	HIS	-	expression tag	UNP A3SNF8
C	377	HIS	-	expression tag	UNP A3SNF8
D	-1	MET	-	expression tag	UNP A3SNF8
D	0	SER	-	expression tag	UNP A3SNF8
D	1	LEU	-	expression tag	UNP A3SNF8
D	370	GLU	-	expression tag	UNP A3SNF8
D	371	GLY	-	expression tag	UNP A3SNF8
D	372	HIS	-	expression tag	UNP A3SNF8
D	373	HIS	-	expression tag	UNP A3SNF8
D	374	HIS	-	expression tag	UNP A3SNF8
D	375	HIS	-	expression tag	UNP A3SNF8
D	376	HIS	-	expression tag	UNP A3SNF8
D	377	HIS	-	expression tag	UNP A3SNF8
E	-1	MET	-	expression tag	UNP A3SNF8
E	0	SER	-	expression tag	UNP A3SNF8
E	1	LEU	-	expression tag	UNP A3SNF8
E	370	GLU	-	expression tag	UNP A3SNF8
E	371	GLY	-	expression tag	UNP A3SNF8
E	372	HIS	-	expression tag	UNP A3SNF8
E	373	HIS	-	expression tag	UNP A3SNF8
E	374	HIS	-	expression tag	UNP A3SNF8
E	375	HIS	-	expression tag	UNP A3SNF8
E	376	HIS	-	expression tag	UNP A3SNF8
E	377	HIS	-	expression tag	UNP A3SNF8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	MET	-	expression tag	UNP A3SNF8
F	0	SER	-	expression tag	UNP A3SNF8
F	1	LEU	-	expression tag	UNP A3SNF8
F	370	GLU	-	expression tag	UNP A3SNF8
F	371	GLY	-	expression tag	UNP A3SNF8
F	372	HIS	-	expression tag	UNP A3SNF8
F	373	HIS	-	expression tag	UNP A3SNF8
F	374	HIS	-	expression tag	UNP A3SNF8
F	375	HIS	-	expression tag	UNP A3SNF8
F	376	HIS	-	expression tag	UNP A3SNF8
F	377	HIS	-	expression tag	UNP A3SNF8
G	-1	MET	-	expression tag	UNP A3SNF8
G	0	SER	-	expression tag	UNP A3SNF8
G	1	LEU	-	expression tag	UNP A3SNF8
G	370	GLU	-	expression tag	UNP A3SNF8
G	371	GLY	-	expression tag	UNP A3SNF8
G	372	HIS	-	expression tag	UNP A3SNF8
G	373	HIS	-	expression tag	UNP A3SNF8
G	374	HIS	-	expression tag	UNP A3SNF8
G	375	HIS	-	expression tag	UNP A3SNF8
G	376	HIS	-	expression tag	UNP A3SNF8
G	377	HIS	-	expression tag	UNP A3SNF8
H	-1	MET	-	expression tag	UNP A3SNF8
H	0	SER	-	expression tag	UNP A3SNF8
H	1	LEU	-	expression tag	UNP A3SNF8
H	370	GLU	-	expression tag	UNP A3SNF8
H	371	GLY	-	expression tag	UNP A3SNF8
H	372	HIS	-	expression tag	UNP A3SNF8
H	373	HIS	-	expression tag	UNP A3SNF8
H	374	HIS	-	expression tag	UNP A3SNF8
H	375	HIS	-	expression tag	UNP A3SNF8
H	376	HIS	-	expression tag	UNP A3SNF8
H	377	HIS	-	expression tag	UNP A3SNF8

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

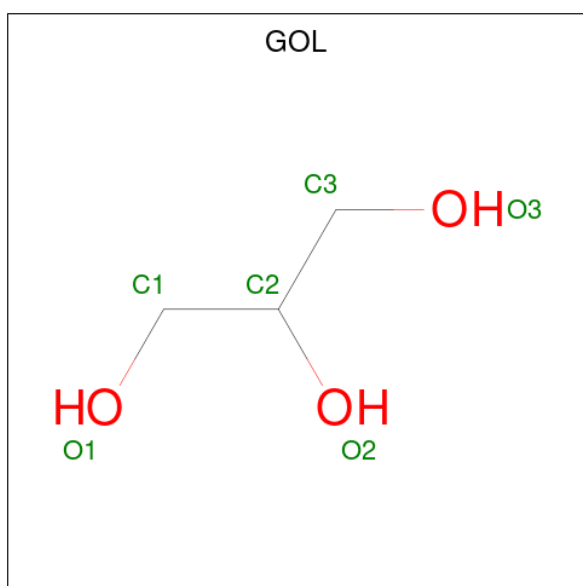
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

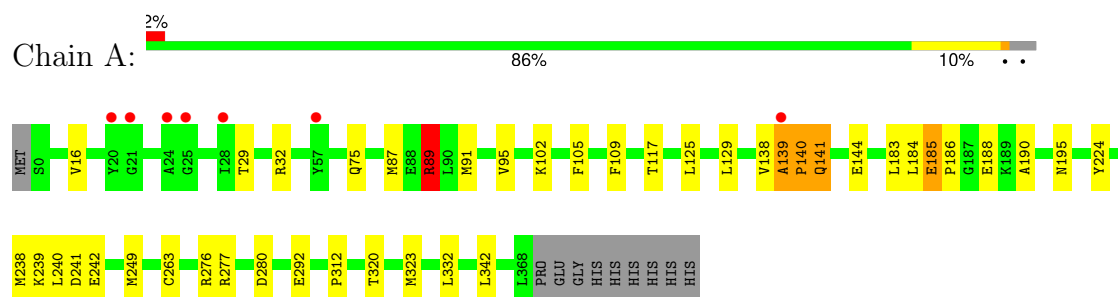
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total	O	0	0
			149	149		
4	B	126	Total	O	0	0
			126	126		
4	C	152	Total	O	0	0
			152	152		
4	D	135	Total	O	0	0
			135	135		
4	E	101	Total	O	0	0
			101	101		
4	F	94	Total	O	0	0
			94	94		
4	G	141	Total	O	0	0
			141	141		
4	H	127	Total	O	0	0
			127	127		



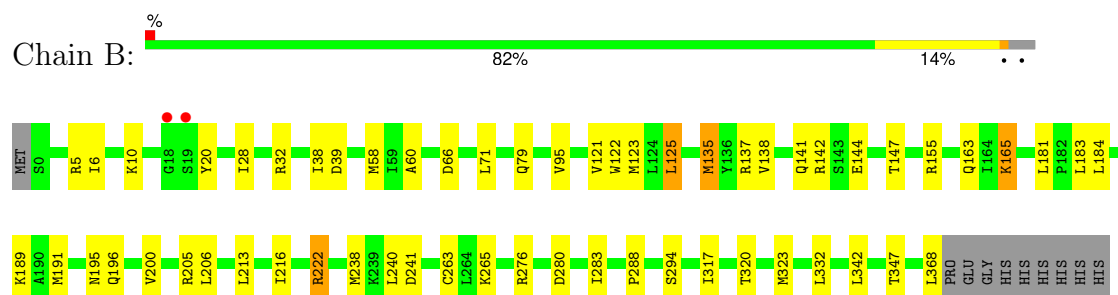
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

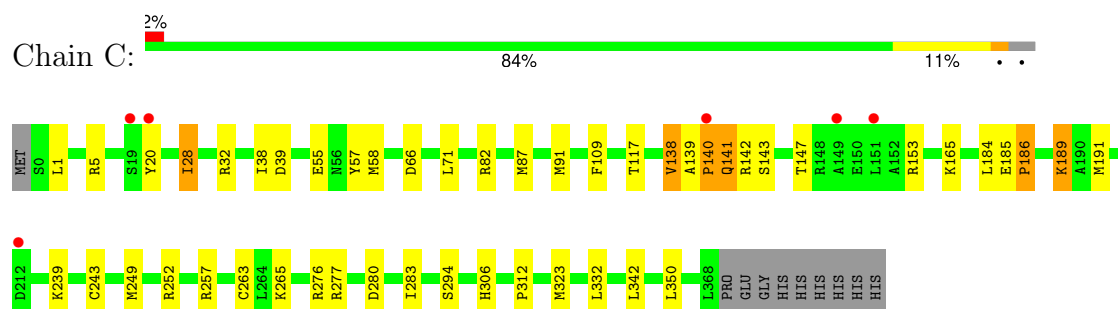
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative



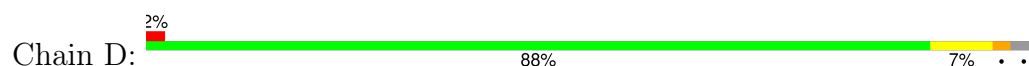
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative

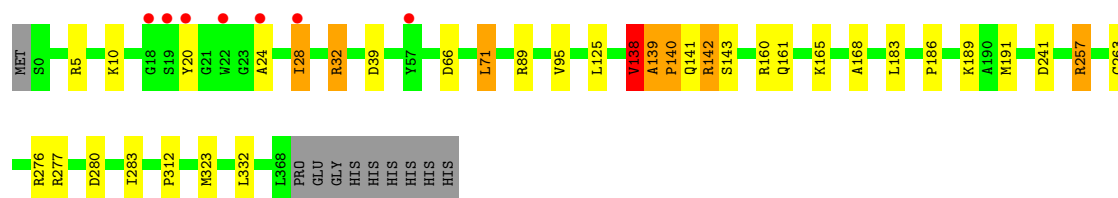


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative

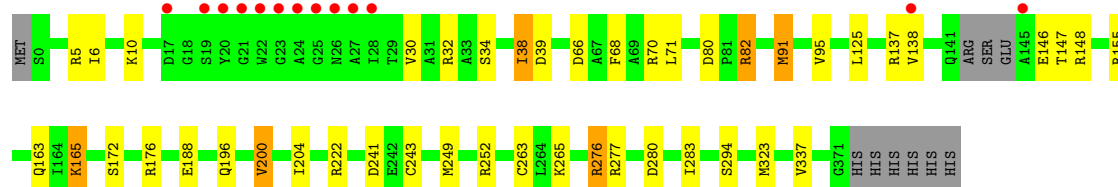
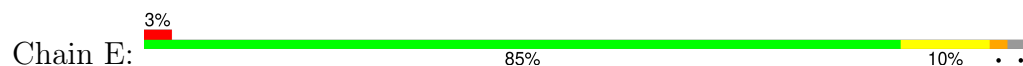


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative

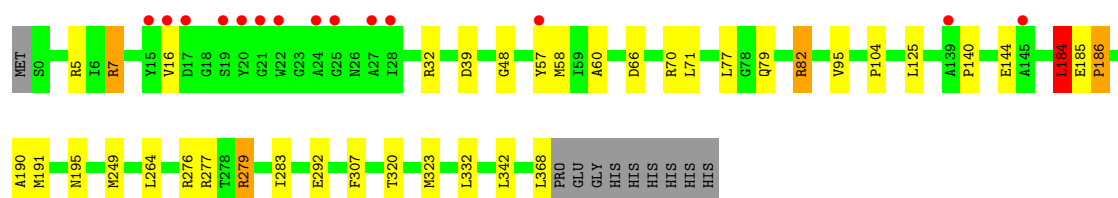
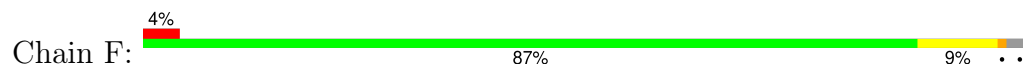




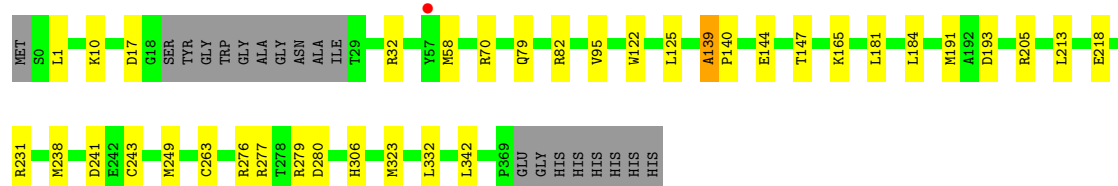
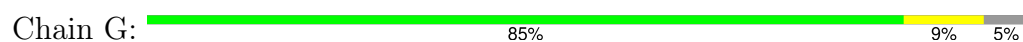
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative



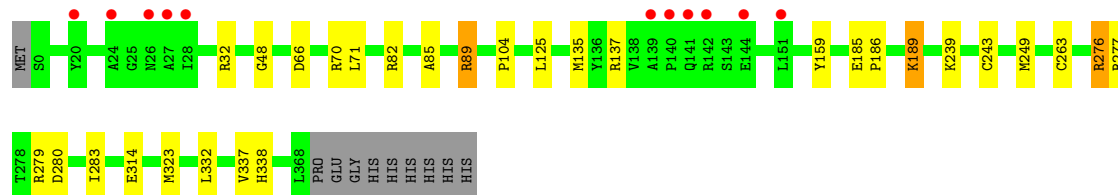
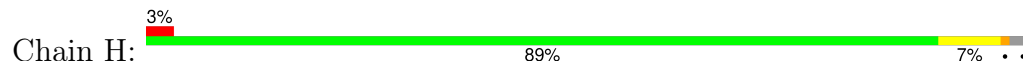
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.41Å 169.22Å 223.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 30.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.00-2.00) 97.9 (30.84-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, $R_{free}$	0.194 , 0.256 0.197 , 0.255	Depositor DCC
$R_{free}$ test set	6360 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 24.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.051 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.96% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL

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	0.41	0/2976	0.66	2/4034 (0.0%)
1	B	0.39	0/2921	0.62	0/3962
1	C	0.42	0/2946	0.63	0/3994
1	D	0.45	0/2994	0.66	1/4056 (0.0%)
1	E	0.39	0/2942	0.61	0/3989
1	F	0.40	0/2915	0.62	1/3955 (0.0%)
1	G	0.41	0/2855	0.61	0/3871
1	H	0.42	0/2946	0.62	0/3994
All	All	0.41	0/23495	0.63	4/31855 (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	A	1	2
1	C	0	1
1	D	0	2
All	All	1	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89[A]	ARG	N-CA-C	5.74	126.51	111.00
1	A	89[B]	ARG	N-CA-C	5.74	126.51	111.00
1	F	184	LEU	CA-CB-CG	5.51	127.97	115.30
1	D	138	VAL	CB-CA-C	-5.42	101.09	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	89[A]	ARG	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ALA	Peptide
1	A	185	GLU	Peptide
1	C	139	ALA	Peptide
1	D	138	VAL	Peptide
1	D	139	ALA	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	2890	0	2852	33	0
1	B	2851	0	2797	21	0
1	C	2872	0	2828	29	0
1	D	2910	0	2877	22	0
1	E	2865	0	2819	21	0
1	F	2850	0	2788	20	0
1	G	2793	0	2744	21	0
1	H	2869	0	2828	16	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
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	16	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	149	0	0	3	0
4	B	126	0	0	1	0
4	C	152	0	0	3	0
4	D	135	0	0	0	0
4	E	101	0	0	0	0
4	F	94	0	0	1	0
4	G	141	0	0	3	0
4	H	127	0	0	1	0
All	All	23975	0	22589	167	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 167 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:185:GLU:HB2	1:A:186:PRO:HD3	1.26	1.09
1:A:185:GLU:HB2	1:A:186:PRO:CD	1.92	1.00
1:A:139:ALA:HB1	1:A:140:PRO:HD3	1.45	0.96
1:C:140:PRO:HG2	1:C:147:THR:HG22	1.52	0.90
1:G:139:ALA:HB1	1:G:140:PRO:HA	1.53	0.88

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	377/379 (100%)	363 (96%)	13 (3%)	1 (0%)	41	37
1	B	371/379 (98%)	358 (96%)	13 (4%)	0	100	100
1	C	373/379 (98%)	357 (96%)	12 (3%)	4 (1%)	14	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	378/379 (100%)	362 (96%)	13 (3%)	3 (1%)	19	13
1	E	371/379 (98%)	356 (96%)	15 (4%)	0	100	100
1	F	370/379 (98%)	353 (95%)	15 (4%)	2 (0%)	29	23
1	G	359/379 (95%)	346 (96%)	12 (3%)	1 (0%)	41	37
1	H	373/379 (98%)	361 (97%)	12 (3%)	0	100	100
All	All	2972/3032 (98%)	2856 (96%)	105 (4%)	11 (0%)	41	30

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	140	PRO
1	C	141	GLN
1	D	140	PRO
1	G	139	ALA
1	A	140	PRO

### 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	298/297 (100%)	283 (95%)	15 (5%)	24	20
1	B	292/297 (98%)	265 (91%)	27 (9%)	9	5
1	C	294/297 (99%)	278 (95%)	16 (5%)	22	18
1	D	298/297 (100%)	281 (94%)	17 (6%)	20	16
1	E	293/297 (99%)	273 (93%)	20 (7%)	16	11
1	F	291/297 (98%)	274 (94%)	17 (6%)	20	15
1	G	287/297 (97%)	273 (95%)	14 (5%)	25	21
1	H	294/297 (99%)	280 (95%)	14 (5%)	25	22
All	All	2347/2376 (99%)	2207 (94%)	140 (6%)	20	14

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	79	GLN
1	G	165	LYS
1	H	89[A]	ARG
1	C	184	LEU
1	C	165	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	195	ASN
1	G	357	ASN
1	H	338	HIS
1	H	141	GLN
1	D	196	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	GOL	F	379	-	5,5,5	0.37	0	5,5,5	0.61	0
3	GOL	A	379	-	5,5,5	0.36	0	5,5,5	0.50	0
3	GOL	A	380	-	5,5,5	0.42	0	5,5,5	0.37	0
3	GOL	D	379	-	5,5,5	0.36	0	5,5,5	0.90	0
3	GOL	G	379	-	5,5,5	0.44	0	5,5,5	0.72	0
3	GOL	C	379	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	H	379	-	5,5,5	0.40	0	5,5,5	0.55	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	GOL	F	379	-	-	2/4/4/4	-
3	GOL	A	379	-	-	0/4/4/4	-
3	GOL	A	380	-	-	4/4/4/4	-
3	GOL	D	379	-	-	2/4/4/4	-
3	GOL	G	379	-	-	2/4/4/4	-
3	GOL	C	379	-	-	4/4/4/4	-
3	GOL	H	379	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	380	GOL	C1-C2-C3-O3
3	A	380	GOL	O2-C2-C3-O3
3	H	379	GOL	O1-C1-C2-C3
3	A	380	GOL	O1-C1-C2-O2
3	C	379	GOL	O2-C2-C3-O3

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	369/379 (97%)	-0.52	7 (1%) 66 65	14, 24, 54, 85	0
1	B	369/379 (97%)	-0.50	2 (0%) 91 90	15, 25, 44, 73	0
1	C	369/379 (97%)	-0.46	6 (1%) 72 70	12, 24, 56, 91	0
1	D	369/379 (97%)	-0.41	7 (1%) 66 65	15, 25, 53, 98	0
1	E	369/379 (97%)	-0.30	13 (3%) 44 43	11, 24, 65, 109	0
1	F	369/379 (97%)	-0.12	14 (3%) 40 39	10, 25, 59, 86	0
1	G	360/379 (94%)	-0.54	1 (0%) 94 93	14, 25, 51, 69	0
1	H	369/379 (97%)	-0.39	11 (2%) 50 49	8, 24, 67, 111	0
All	All	2943/3032 (97%)	-0.40	61 (2%) 63 62	8, 24, 57, 111	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	25	GLY	8.2
1	E	24	ALA	6.5
1	E	28	ILE	6.5
1	E	20	TYR	5.9
1	F	27	ALA	5.9

### 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 monosaccharides 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
3	GOL	C	379	6/6	0.94	0.15	21,51,64,71	0
3	GOL	D	379	6/6	0.94	0.13	20,43,49,54	0
3	GOL	G	379	6/6	0.94	0.14	26,34,43,58	0
3	GOL	A	379	6/6	0.95	0.18	31,59,64,64	0
3	GOL	F	379	6/6	0.96	0.17	21,43,55,59	0
3	GOL	H	379	6/6	0.96	0.24	25,47,62,71	0
3	GOL	A	380	6/6	0.97	0.22	20,34,59,92	0
2	MG	C	378	1/1	0.98	0.03	13,13,13,13	0
2	MG	D	378	1/1	0.98	0.04	20,20,20,20	0
2	MG	E	378	1/1	0.98	0.04	24,24,24,24	0
2	MG	F	378	1/1	0.98	0.03	30,30,30,30	0
2	MG	H	378	1/1	0.98	0.03	22,22,22,22	0
2	MG	A	378	1/1	0.98	0.03	23,23,23,23	0
2	MG	B	378	1/1	0.99	0.02	22,22,22,22	0
2	MG	G	378	1/1	0.99	0.05	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.