wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2017 – 11:40 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 : unknown

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*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
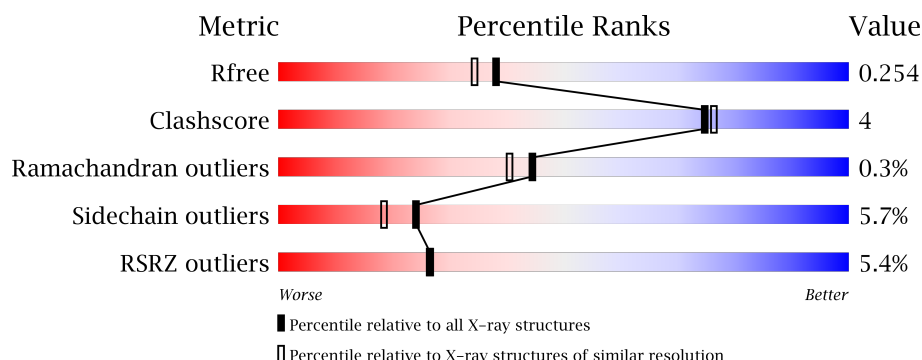Validation Pipeline (wwPDB-VP) : rb-20030345

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	Percentile Ranks	Value
Rfree		0.254
Clashscore		4
Ramachandran outliers		0.3%
Sidechain outliers		5.7%
RSRZ outliers		5.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	5% 86% 10% • •
1	B	379	.% 82% 14% • •
1	C	379	4% 84% 11% • •
1	D	379	5% 88% 7% • •
1	E	379	7% 85% 10% • •

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Mol	Chain	Length	Quality of chain
1	F	379	9% ▬▬ 87% 9% ··
1	G	379	3% ▬ 85% 9% 5%
1	H	379	7% ▬▬ 89% 7% ··

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	380	-	-	-	X
3	GOL	C	379	-	-	-	X
3	GOL	G	379	-	-	-	X

2 Entry composition (i)

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

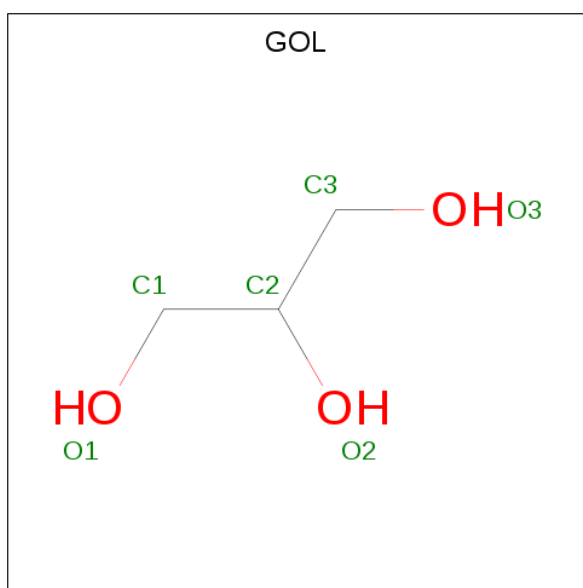- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

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

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

- Molecule 4 is water.

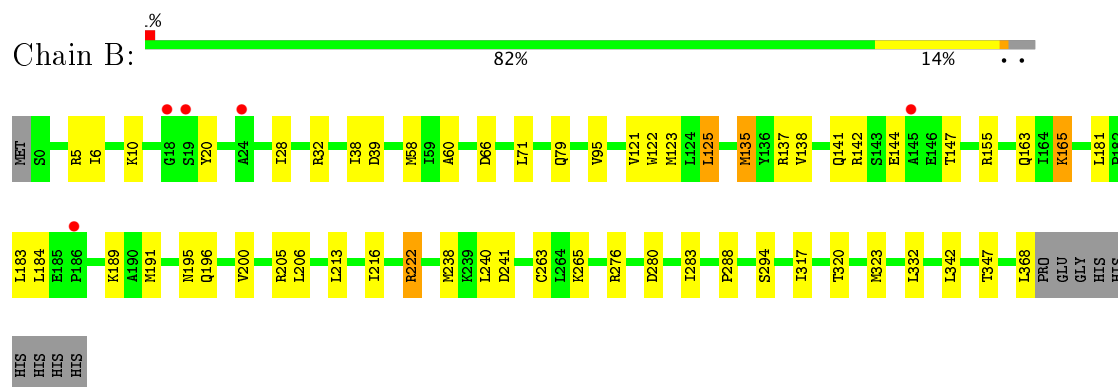| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total 149	O 149	0	0
4	B	126	Total 126	O 126	0	0
4	C	152	Total 152	O 152	0	0
4	D	135	Total 135	O 135	0	0
4	E	101	Total 101	O 101	0	0
4	F	94	Total 94	O 94	0	0
4	G	141	Total 141	O 141	0	0
4	H	127	Total 127	O 127	0	0

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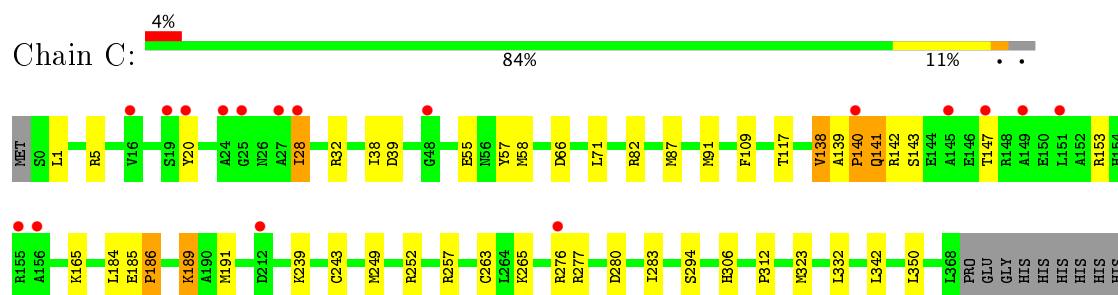
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative
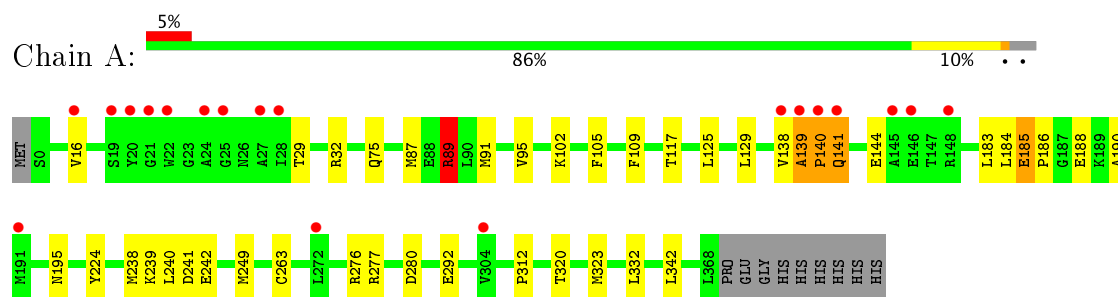
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative

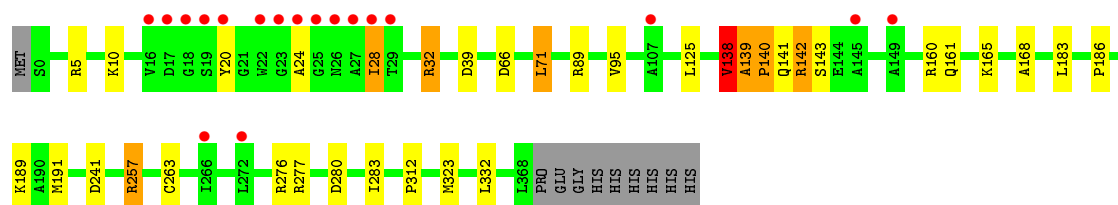- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative

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

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

Chain E:
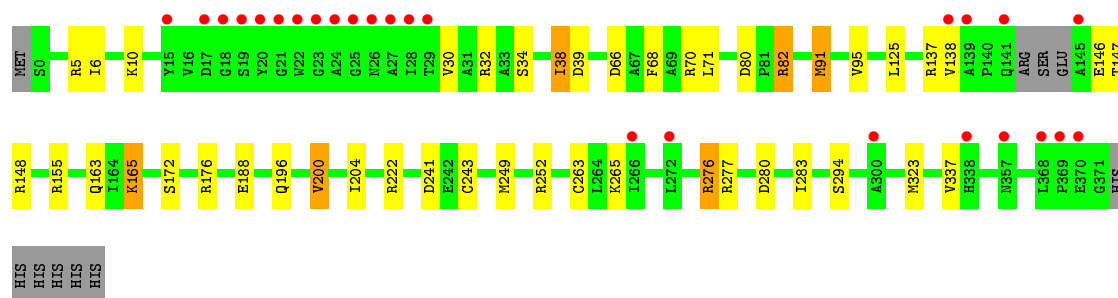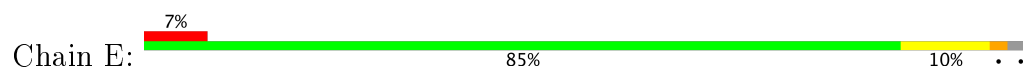

- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative
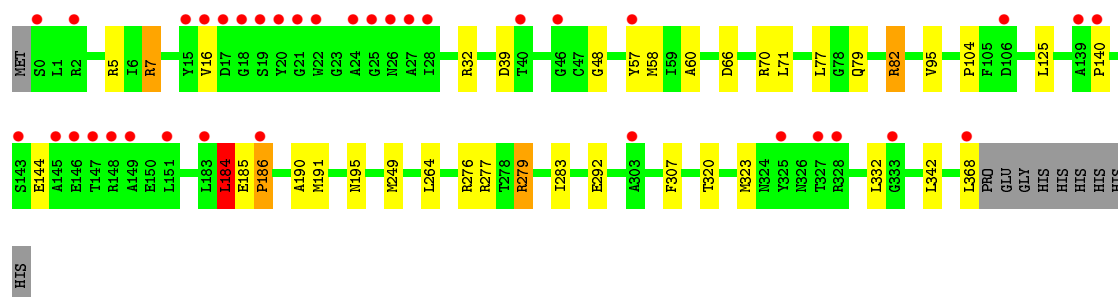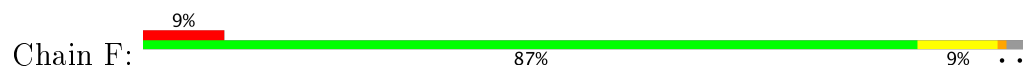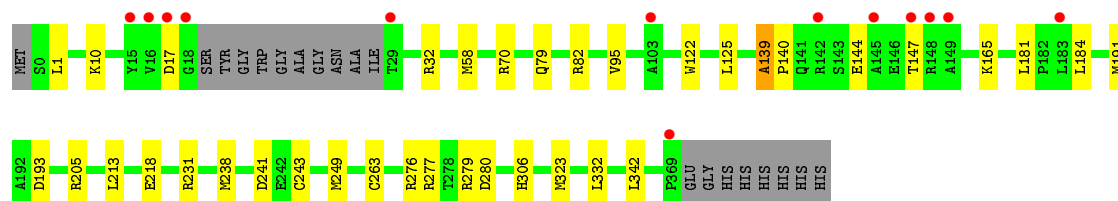
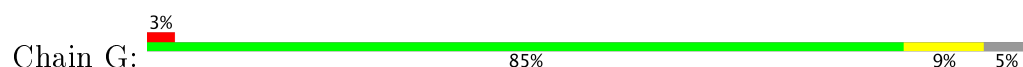Chain F:

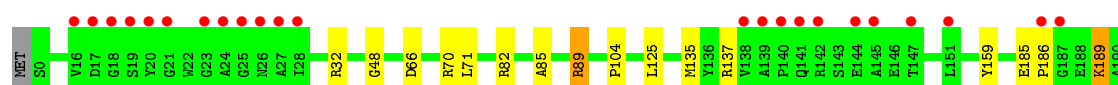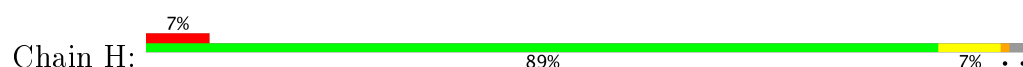- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative

Chain G:

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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	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
$<I/\sigma(I)>$ [1]	1.41 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.194 , 0.256 0.197 , 0.254	Depositor DCC
R_{free} test set	6351 reflections (3.11%)	DCC
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.7	EDS
L-test for twinning [2]	$<\lvert L\rvert> = 0.47, <L^2> = 0.30$	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^2)	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.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<\lvert L\rvert>$, $<L^2>$ 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: GOL, 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	0.41	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(^{o})	Ideal(^{o})
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 (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	377/379 (100%)	363 (96%)	13 (3%)	1 (0%)	44	40
1	B	371/379 (98%)	358 (96%)	13 (4%)	0	100	100
1	C	373/379 (98%)	357 (96%)	12 (3%)	4 (1%)	17	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	378/379 (100%)	362 (96%)	13 (3%)	3 (1%)	22	15
1	E	371/379 (98%)	356 (96%)	15 (4%)	0	100	100
1	F	370/379 (98%)	353 (95%)	15 (4%)	2 (0%)	32	26
1	G	359/379 (95%)	346 (96%)	12 (3%)	1 (0%)	44	40
1	H	373/379 (98%)	361 (97%)	12 (3%)	0	100	100
All	All	2972/3032 (98%)	2856 (96%)	105 (4%)	11 (0%)	44	33

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 (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	298/297 (100%)	283 (95%)	15 (5%)	28	23
1	B	292/297 (98%)	265 (91%)	27 (9%)	11	6
1	C	294/297 (99%)	278 (95%)	16 (5%)	26	20
1	D	298/297 (100%)	281 (94%)	17 (6%)	24	18
1	E	293/297 (99%)	273 (93%)	20 (7%)	18	13
1	F	291/297 (98%)	274 (94%)	17 (6%)	23	18
1	G	287/297 (97%)	273 (95%)	14 (5%)	29	24
1	H	294/297 (99%)	280 (95%)	14 (5%)	30	25
All	All	2347/2376 (99%)	2207 (94%)	140 (6%)	24	17

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

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Mol	Chain	Res	Type
1	D	138	VAL
1	E	66	ASP
1	H	82	ARG
1	D	142	ARG
1	D	257[A]	ARG

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

Mol	Chain	Res	Type
1	E	75	GLN
1	E	79	GLN
1	G	306	HIS
1	D	306	HIS
1	D	357	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 carbohydrates 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	A	379	-	5,5,5	0.34	0	5,5,5	0.43	0
3	GOL	A	380	-	5,5,5	0.40	0	5,5,5	0.31	0
3	GOL	C	379	-	5,5,5	0.31	0	5,5,5	0.21	0
3	GOL	D	379	-	5,5,5	0.35	0	5,5,5	0.79	0
3	GOL	F	379	-	5,5,5	0.36	0	5,5,5	0.52	0
3	GOL	G	379	-	5,5,5	0.44	0	5,5,5	0.61	0
3	GOL	H	379	-	5,5,5	0.40	0	5,5,5	0.47	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	A	379	-	-	0/4/4/4	0/0/0/0
3	GOL	A	380	-	-	0/4/4/4	0/0/0/0
3	GOL	C	379	-	-	0/4/4/4	0/0/0/0
3	GOL	D	379	-	-	0/4/4/4	0/0/0/0
3	GOL	F	379	-	-	0/4/4/4	0/0/0/0
3	GOL	G	379	-	-	0/4/4/4	0/0/0/0
3	GOL	H	379	-	-	0/4/4/4	0/0/0/0

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.

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, 95th 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^2)	Q<0.9
1	A	369/379 (97%)	0.00	19 (5%)	29	29	14, 24, 54, 85	0
1	B	369/379 (97%)	-0.10	5 (1%)	75	75	15, 25, 44, 73	0
1	C	369/379 (97%)	-0.01	17 (4%)	33	33	12, 24, 56, 91	0
1	D	369/379 (97%)	0.06	18 (4%)	30	30	15, 25, 53, 98	0
1	E	369/379 (97%)	0.21	26 (7%)	17	17	11, 24, 65, 109	0
1	F	369/379 (97%)	0.52	36 (9%)	8	8	10, 25, 59, 86	0
1	G	360/379 (94%)	-0.04	13 (3%)	43	44	14, 25, 51, 69	0
1	H	369/379 (97%)	0.11	25 (6%)	18	18	8, 24, 67, 111	0
All	All	2943/3032 (97%)	0.09	159 (5%)	26	26	8, 25, 57, 111	0

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	28	ILE	12.0
1	F	27	ALA	9.3
1	E	25	GLY	8.7
1	E	24	ALA	8.4
1	E	21	GLY	7.9

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 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, 95th 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^2)	Q<0.9
3	GOL	A	380	6/6	0.93	0.31	17.65	20,34,59,92	0
3	GOL	G	379	6/6	0.94	0.20	9.81	26,34,43,58	0
3	GOL	C	379	6/6	0.91	0.20	3.23	21,51,64,71	0
3	GOL	H	379	6/6	0.93	0.27	1.87	25,47,62,71	0
3	GOL	A	379	6/6	0.91	0.21	0.77	31,59,64,64	0
3	GOL	D	379	6/6	0.90	0.19	0.57	20,43,49,54	0
3	GOL	F	379	6/6	0.94	0.18	0.54	21,43,55,59	0
2	MG	B	378	1/1	0.99	0.04	-1.93	22,22,22,22	0
2	MG	G	378	1/1	0.98	0.05	-2.34	19,19,19,19	0
2	MG	E	378	1/1	0.97	0.05	-2.35	24,24,24,24	0
2	MG	C	378	1/1	0.98	0.05	-2.40	13,13,13,13	0
2	MG	A	378	1/1	0.99	0.07	-2.94	23,23,23,23	0
2	MG	D	378	1/1	0.98	0.06	-3.51	20,20,20,20	0
2	MG	H	378	1/1	0.97	0.04	-3.63	22,22,22,22	0
2	MG	F	378	1/1	0.97	0.04	-3.77	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.