WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)
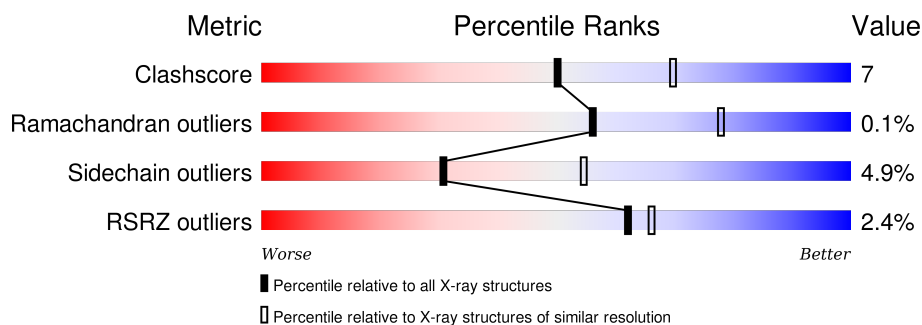
Feb 1, 2016 – 05:41 PM GMT

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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 2.50 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
Clashscore		7
Ramachandran outliers		0.1%
Sidechain outliers		4.9%
RSRZ outliers		2.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
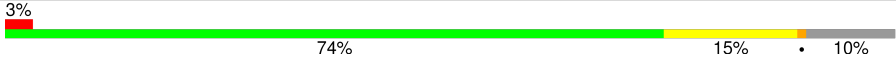
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	429	3% 74% 15% • 10%
1	B	429	2% 73% 16% • 10%
1	C	429	2% 76% 13% • 10%
1	D	429	3% 74% 16% • 8%
1	E	429	2% 74% 14% • 10%
1	F	429	2% 73% 17% • 10%
1	G	429	2% 74% 15% 10%

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Mol	Chain	Length	Quality of chain
1	H	429	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 24704 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	388	Total	C	N	O	S	0	0	0
			2939	1871	518	535	15			
1	B	386	Total	C	N	O	S	0	0	0
			2922	1861	515	532	14			
1	C	386	Total	C	N	O	S	0	0	0
			2922	1861	515	532	14			
1	D	393	Total	C	N	O	S	0	2	0
			2987	1901	527	542	17			
1	E	388	Total	C	N	O	S	0	0	0
			2938	1871	517	534	16			
1	F	386	Total	C	N	O	S	0	0	0
			2922	1861	515	532	14			
1	G	386	Total	C	N	O	S	0	2	0
			2935	1870	518	533	14			
1	H	388	Total	C	N	O	S	0	0	0
			2938	1871	517	534	16			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q28RT0
A	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
A	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
A	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
A	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
A	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
A	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
A	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
A	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
A	415	SER	-	EXPRESSION TAG	UNP Q28RT0
A	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
A	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
A	418	HIS	-	EXPRESSION TAG	UNP Q28RT0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
A	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
A	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
A	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
A	423	SER	-	EXPRESSION TAG	UNP Q28RT0
A	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
A	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
A	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
A	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
A	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
A	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
B	1	MET	-	EXPRESSION TAG	UNP Q28RT0
B	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
B	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
B	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
B	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
B	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
B	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
B	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
B	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
B	415	SER	-	EXPRESSION TAG	UNP Q28RT0
B	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	418	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
B	423	SER	-	EXPRESSION TAG	UNP Q28RT0
B	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
B	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
B	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
B	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
B	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
C	1	MET	-	EXPRESSION TAG	UNP Q28RT0
C	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
C	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
C	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
C	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
C	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
C	412	TYR	-	EXPRESSION TAG	UNP Q28RT0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
C	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
C	415	SER	-	EXPRESSION TAG	UNP Q28RT0
C	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	418	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
C	423	SER	-	EXPRESSION TAG	UNP Q28RT0
C	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
C	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
C	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
C	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
C	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
D	1	MET	-	EXPRESSION TAG	UNP Q28RT0
D	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
D	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
D	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
D	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
D	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
D	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
D	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
D	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
D	415	SER	-	EXPRESSION TAG	UNP Q28RT0
D	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	418	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
D	423	SER	-	EXPRESSION TAG	UNP Q28RT0
D	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
D	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
D	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
D	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
D	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
E	1	MET	-	EXPRESSION TAG	UNP Q28RT0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
E	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
E	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
E	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
E	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
E	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
E	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
E	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
E	415	SER	-	EXPRESSION TAG	UNP Q28RT0
E	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	418	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
E	423	SER	-	EXPRESSION TAG	UNP Q28RT0
E	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
E	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
E	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
E	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
E	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
F	1	MET	-	EXPRESSION TAG	UNP Q28RT0
F	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
F	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
F	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
F	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
F	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
F	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
F	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
F	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
F	415	SER	-	EXPRESSION TAG	UNP Q28RT0
F	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
F	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
F	418	HIS	-	EXPRESSION TAG	UNP Q28RT0
F	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
F	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
F	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
F	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
F	423	SER	-	EXPRESSION TAG	UNP Q28RT0
F	424	HIS	-	EXPRESSION TAG	UNP Q28RT0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
F	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
F	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
F	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
F	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
G	1	MET	-	EXPRESSION TAG	UNP Q28RT0
G	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
G	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
G	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
G	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
G	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
G	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
G	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
G	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
G	415	SER	-	EXPRESSION TAG	UNP Q28RT0
G	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	418	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
G	423	SER	-	EXPRESSION TAG	UNP Q28RT0
G	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
G	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
G	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
G	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
G	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
H	1	MET	-	EXPRESSION TAG	UNP Q28RT0
H	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
H	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
H	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
H	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
H	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
H	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
H	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
H	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
H	415	SER	-	EXPRESSION TAG	UNP Q28RT0
H	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
H	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
H	418	HIS	-	EXPRESSION TAG	UNP Q28RT0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
H	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
H	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
H	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
H	423	SER	-	EXPRESSION TAG	UNP Q28RT0
H	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
H	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
H	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
H	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
H	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
H	429	LYS	-	EXPRESSION TAG	UNP Q28RT0

- Molecule 2 is water.

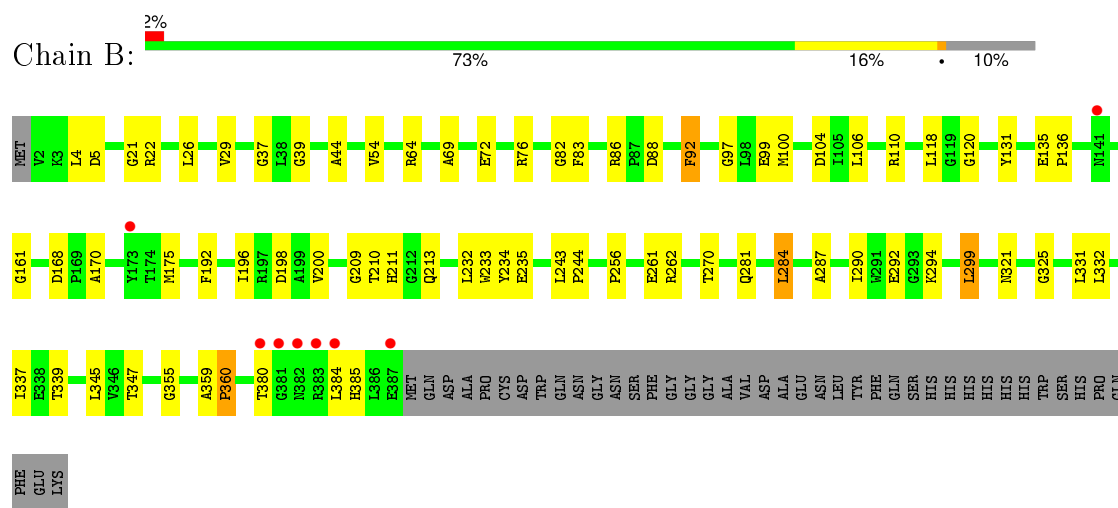| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	157	Total 157	O 157	0	0
2	B	147	Total 147	O 147	0	0
2	C	157	Total 157	O 157	0	0
2	D	145	Total 145	O 145	0	0
2	E	157	Total 157	O 157	0	0
2	F	141	Total 141	O 141	0	0
2	G	139	Total 139	O 139	0	0
2	H	158	Total 158	O 158	0	0

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.
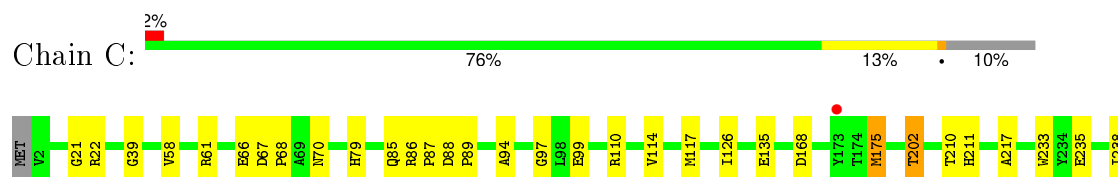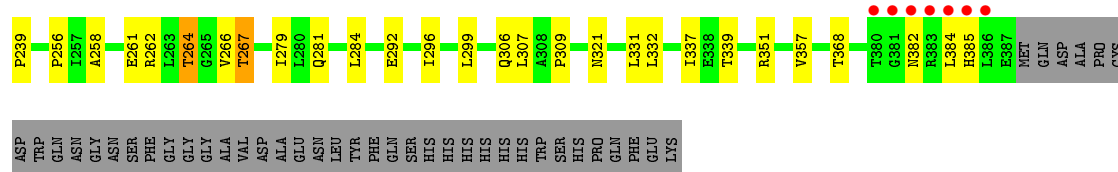
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

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- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

P239 P256 I257 A258 E261 R262 L263 T264 G265 V266 T267 I279 L280 Q281 L284 E292 I296 I299 Q306 L307 A308 P309 N321 L331 L332 I337 E338 T339 R351 V357 T368 T380 G381 N382 R383 L384 H385 L386 E387 MET GLN ASP ALA PRO CYS

ASP TRP GLN ASN GLY ASN SER PHE GLY GLY GLY ALA VAL ASP ALA ASN LEU TYR PHE GLN SER HIS HIS HIS HIS HIS TRP SER PRO GLN PHE GLU LYS

- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain D:

3%

74% 16% • 8%

M1 V2 K3 L4 L7 G20 G21 R22 Y23 V27 G34 L38 G39 A44 G45 V46 G47 P48 T52 H56 P68 A69 N70 F83 R86 G97 L98 E99 W103 G107 D111 C112 A116 N123 I126 Y131 L132 Y133 N141

E148 R157 F167 D168 P169 A170 Y173 T174 M175 C193 R197 T202 D205 T210 Q213 K224 L232 W233 Y234 E235 P256 I257 A258 E261 I279 L284 W291 K295 A302 V316 V322 G325 V326 L331 L332 I337

G364 I367 T368 L369 G381 N382 R383 L384 H385 L386 E387 M388 Q389 D390 A391 P392 C393 ASP TRP GLN ASN GLY ASN SER PHE GLY GLY GLY ALA VAL ASP ALA ASN LEU TYR PHE GLN SER HIS HIS HIS HIS HIS TRP SER PRO GLN PHE GLU LYS
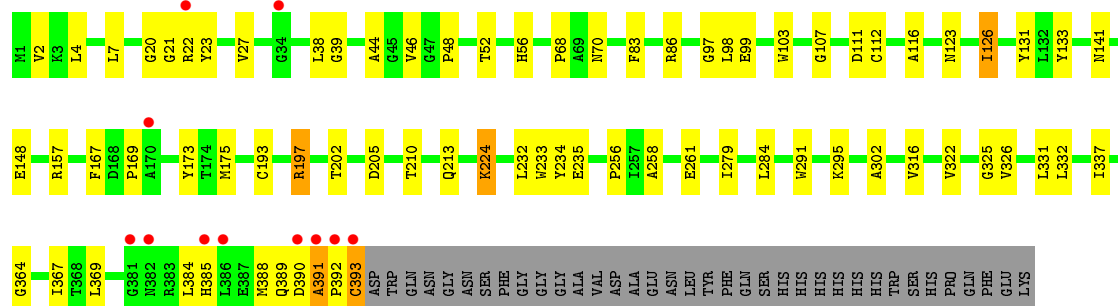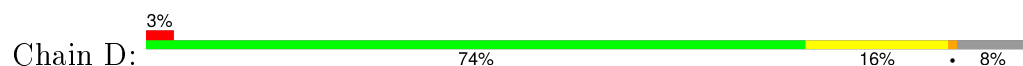
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain E:

2%

74% 14% • 10%

M1 L4 D5 T6 L7 P17 G18 W19 G20 G21 V29 G34 G39 A44 I55 R61 A69 F83 T84 Q85 R86 P87 D88 P89 F92 G97 L106 G107 R110 D111 C112 P113 M117 G120 K121 M122 R127 E135 P136 R157

P172 Y173 T174 M175 R176 R197 D198 T210 Q213 A217 K224 Y229 D230 W233 Y234 I238 P239 N242 G245 E248 R262 T270 H274 R278 I279 L280 G288 K294 L299 A300 A308 P309 H323 P329 M333 V334 G348

T368 N382 R383 L384 H385 L386 E387 M388 GLN ASP ALA PRO CYS ASP TRP GLN ASN GLY ASN SER PHE GLY GLY GLY ALA VAL ASP ALA GLU ASN LEU TYR PHE GLN SER HIS HIS HIS HIS HIS TRP SER HIS PRO GLN PHE GLU LYS
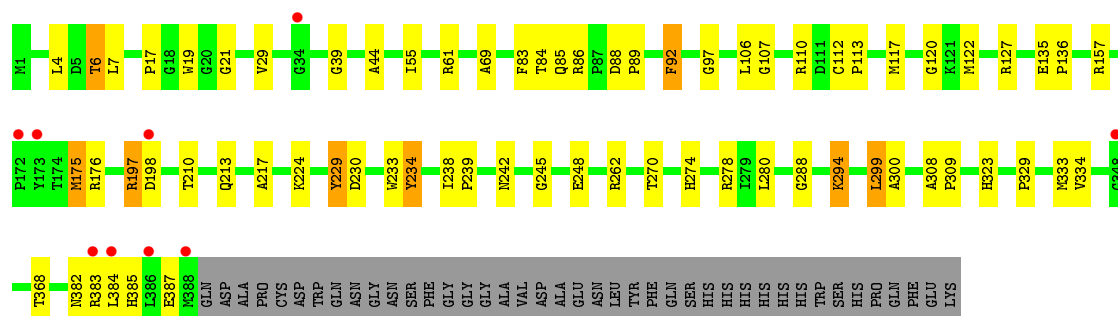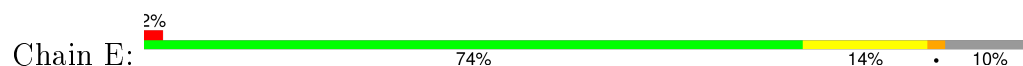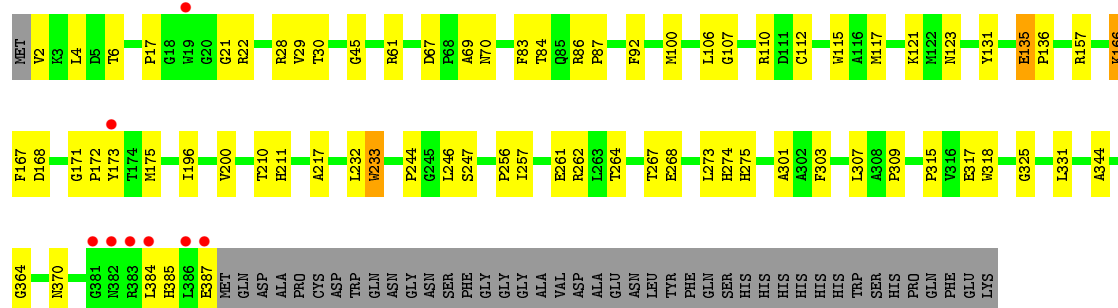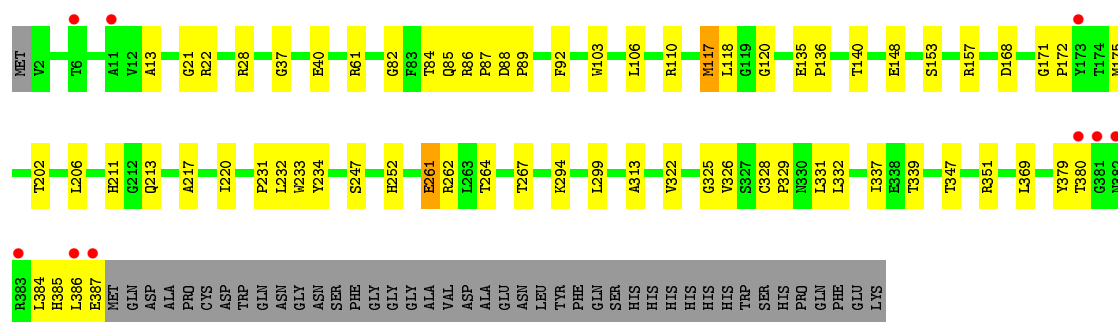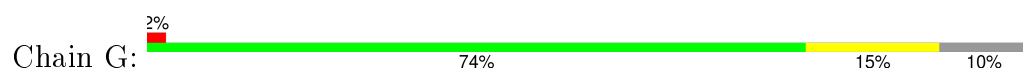
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain F:

2%

73% 17% • 10%

MET V2 K3 L4 D5 T6 P17 G18 W19 G20 G21 R22 R28 V29 T30 G45 R61 D67 P68 A69 N70 F83 T84 Q85 R86 P87 F92 M100 L106 G107 R110 D111 C112 W115 A116 M117 K121 M122 N123 Y131 E135 P136 R157 K166

F167 D168 G171 P172 Y173 T174 M175 I196 V200 T210 E211 A217 L232 W233 P244 G245 L246 S247 P256 I257 E261 R262 L263 T264 T267 E268 L273 H274 H275 A301 A302 F303 L307 A308 P309 P315 V316 E317 W318 G325 L331 A344

G364 N370 G381 N382 R383 L384 H385 L386 E387 MET GLN ASP ALA PRO CYS ASP TRP GLN ASN GLY ASN SER PHE GLY GLY GLY ALA VAL ASP ALA GLU ASN LEU TYR PHE GLN SER HIS HIS HIS HIS HIS TRP SER HIS PRO GLN PHE GLU LYS
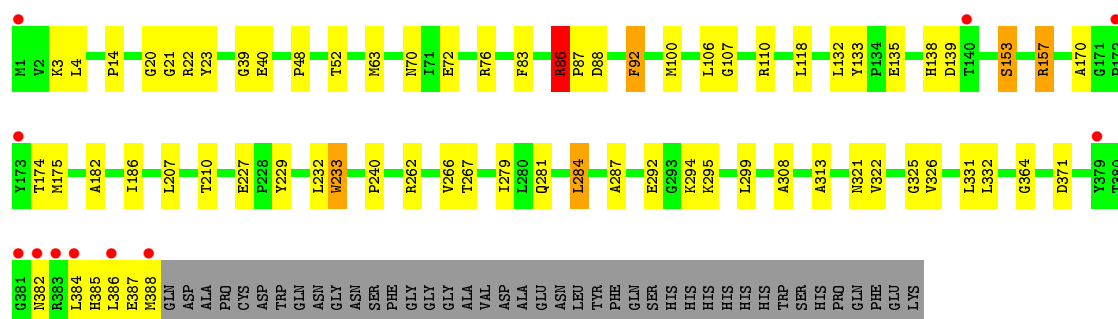
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain G:

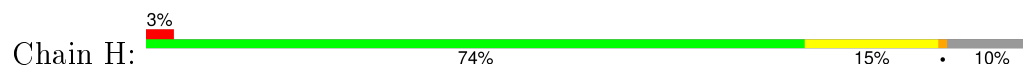• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	126.91Å 126.63Å 126.78Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	44.88 – 2.50 44.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.88-2.50) 98.7 (44.88-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.41 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.211 , 0.245 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.0	EDS
Estimated twinning fraction	0.747 for H, K, L 0.091 for H, -K, -L 0.083 for -H, -L, -K 0.079 for -H, L, K 0.000 for -l,k,h 0.000 for -k,-h,-l 0.000 for k,h,-l 0.248 for -h,l,k 0.259 for -h,-l,-k 0.000 for k,l,h 0.000 for l,h,k 0.000 for k,-l,-h 0.000 for l,-h,-k 0.260 for -h,-k,l 0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.747 for H, K, L 0.091 for H, -K, -L 0.083 for -H, -L, -K 0.079 for -H, L, K	Depositor
L-test for twinning[2]	$< |L| > = 0.53, < L^2 > = 0.37$	Xtriage
Outliers	2 of 138036 reflections (0.001%)	Xtriage

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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Property	Value	Source
F_o,F_c correlation	0.85	EDS
Total number of atoms	24704	wwPDB-VP
Average B, all atoms ($Å^2$)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality (i)

5.1 Standard geometry (i)

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	0.55	2/3026 (0.1%)	0.62	0/4136
1	B	0.48	1/3009 (0.0%)	0.62	2/4114 (0.0%)
1	C	0.46	0/3009	0.59	0/4114
1	D	0.55	0/3083	0.66	4/4214 (0.1%)
1	E	0.49	1/3025 (0.0%)	0.62	2/4134 (0.0%)
1	F	0.55	0/3009	0.60	0/4114
1	G	0.48	0/3029	0.60	0/4141
1	H	0.52	1/3025 (0.0%)	0.61	3/4134 (0.1%)
All	All	0.51	5/24215 (0.0%)	0.62	11/33101 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	229	TYR	CE1-CZ	-5.61	1.31	1.38
1	A	16	PRO	N-CD	5.60	1.55	1.47
1	A	17	PRO	N-CD	5.50	1.55	1.47
1	B	360	PRO	N-CD	5.14	1.55	1.47
1	H	87	PRO	N-CD	5.13	1.55	1.47

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	ARG	NE-CZ-NH2	8.46	124.53	120.30
1	E	157	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	D	157	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	H	157	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	E	230	ASP	CB-CG-OD1	5.69	123.42	118.30

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	2939	0	2857	46	0
1	B	2922	0	2840	40	0
1	C	2922	0	2840	44	0
1	D	2987	0	2904	55	0
1	E	2938	0	2861	59	0
1	F	2922	0	2840	45	0
1	G	2935	0	2855	40	0
1	H	2938	0	2861	40	0
2	A	157	0	0	2	0
2	B	147	0	0	0	0
2	C	157	0	0	1	0
2	D	145	0	0	1	0
2	E	157	0	0	2	0
2	F	141	0	0	1	0
2	G	139	0	0	0	0
2	H	158	0	0	0	0
All	All	24704	0	22858	323	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 7.

The worst 5 of 323 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:LEU:HD22	1:E:29:VAL:HG11	1.46	0.95
1:C:126:ILE:HG23	1:C:331:LEU:HD21	1.54	0.89
1:A:83:PHE:CZ	1:C:211:HIS:HD2	1.90	0.89
1:E:217:ALA:HB1	1:F:256:PRO:HB3	1.56	0.87
1:D:389:GLN:OE1	1:D:391:ALA:HB3	1.75	0.86

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	386/429 (90%)	362 (94%)	23 (6%)	1 (0%)	46	68
1	B	384/429 (90%)	362 (94%)	22 (6%)	0	100	100
1	C	384/429 (90%)	360 (94%)	24 (6%)	0	100	100
1	D	393/429 (92%)	381 (97%)	12 (3%)	0	100	100
1	E	386/429 (90%)	366 (95%)	20 (5%)	0	100	100
1	F	384/429 (90%)	368 (96%)	15 (4%)	1 (0%)	46	68
1	G	386/429 (90%)	368 (95%)	18 (5%)	0	100	100
1	H	386/429 (90%)	371 (96%)	15 (4%)	0	100	100
All	All	3089/3432 (90%)	2938 (95%)	149 (5%)	2 (0%)	56	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	GLY
1	F	45	GLY

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	293/327 (90%)	278 (95%)	15 (5%)	29	52
1	B	291/327 (89%)	277 (95%)	14 (5%)	31	55
1	C	291/327 (89%)	279 (96%)	12 (4%)	37	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	299/327 (91%)	283 (95%)	16 (5%)	27	49
1	E	293/327 (90%)	280 (96%)	13 (4%)	35	60
1	F	291/327 (89%)	275 (94%)	16 (6%)	27	48
1	G	293/327 (90%)	277 (94%)	16 (6%)	27	48
1	H	293/327 (90%)	280 (96%)	13 (4%)	35	60
All	All	2344/2616 (90%)	2229 (95%)	115 (5%)	31	55

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	234	TYR
1	E	234	TYR
1	H	153	SER
1	D	261	GLU
1	E	85	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	382	ASN
1	C	385	HIS
1	G	310	HIS
1	C	211	HIS
1	E	271	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	388/429 (90%)	0.03	11 (2%)	56	61	21, 29, 42, 75	0
1	B	386/429 (89%)	-0.05	8 (2%)	67	71	20, 28, 39, 73	0
1	C	386/429 (89%)	-0.04	8 (2%)	67	71	20, 27, 39, 69	0
1	D	393/429 (91%)	0.07	11 (2%)	56	61	20, 28, 45, 86	0
1	E	388/429 (90%)	0.04	9 (2%)	64	67	21, 29, 41, 69	0
1	F	386/429 (89%)	-0.03	8 (2%)	67	71	21, 28, 41, 81	0
1	G	386/429 (89%)	-0.01	9 (2%)	64	67	19, 27, 39, 81	0
1	H	388/429 (90%)	0.02	11 (2%)	56	61	20, 28, 42, 64	0
All	All	3101/3432 (90%)	0.00	75 (2%)	62	66	19, 28, 41, 86	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	173	TYR	5.5
1	C	381	GLY	5.3
1	A	386	LEU	5.2
1	G	386	LEU	5.0
1	D	381	GLY	4.9

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.