



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 09:05 PM UTC

PDB ID : 3DFY / pdb\_00003dfy  
Title : Crystal structure of apo dipeptide epimerase from *Thermotoga maritima*  
Authors : Fedorov, A.A.; Fedorov, E.V.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.  
Deposited on : 2008-06-12  
Resolution : 2.10 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

<http://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 : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

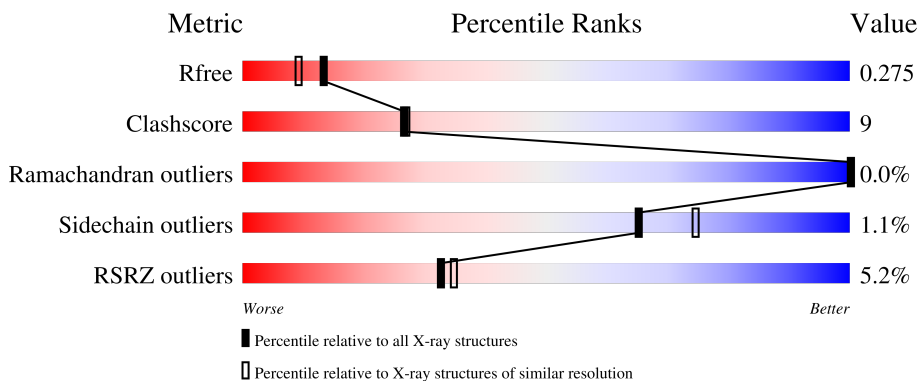
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	345	 4% 75% 22% ..
1	B	345	 4% 76% 19% ..
1	C	345	 6% 78% 19% ..
1	D	345	 6% 72% 23% ..
1	E	345	 6% 70% 23% ..

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Mol	Chain	Length	Quality of chain	
1	F	345	5%	75% 20% ..
1	G	345	4%	69% 24% . .
1	H	345	3%	77% 17% . .
1	I	345	5%	76% 21% . .
1	J	345	6%	76% 19% . .
1	K	345	5%	68% 26% . .
1	L	345	4%	75% 20% . .
1	M	345	7%	74% 23% . .
1	N	345	6%	73% 23% .
1	O	345	5%	73% 22% . .
1	P	345	4%	75% 19% . .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 43115 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 Muconate cycloisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2660	1689	457	504	10	0	0	0
1	B	332	2622	1664	450	498	10	0	0	0
1	C	338	2660	1689	457	504	10	0	0	0
1	D	332	2622	1664	450	498	10	0	0	0
1	E	330	2606	1653	447	496	10	0	0	0
1	F	333	2628	1667	451	500	10	0	0	0
1	G	330	2606	1653	447	496	10	0	0	0
1	H	331	2615	1659	449	497	10	0	0	0
1	I	338	2660	1689	457	504	10	0	0	0
1	J	331	2615	1659	449	497	10	0	0	0
1	K	330	2606	1653	447	496	10	0	0	0
1	L	331	2612	1656	448	498	10	0	0	0
1	M	338	2660	1689	457	504	10	0	0	0
1	N	332	2621	1662	450	499	10	0	0	0
1	O	331	2612	1656	448	498	10	0	0	0
1	P	332	2622	1664	450	498	10	0	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: 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
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	L	1	Total Mg 1 1	0	0
2	M	1	Total Mg 1 1	0	0
2	N	1	Total Mg 1 1	0	0
2	O	1	Total Mg 1 1	0	0
2	P	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	83	Total O 83 83	0	0
3	B	73	Total O 73 73	0	0
3	C	67	Total O 67 67	0	0

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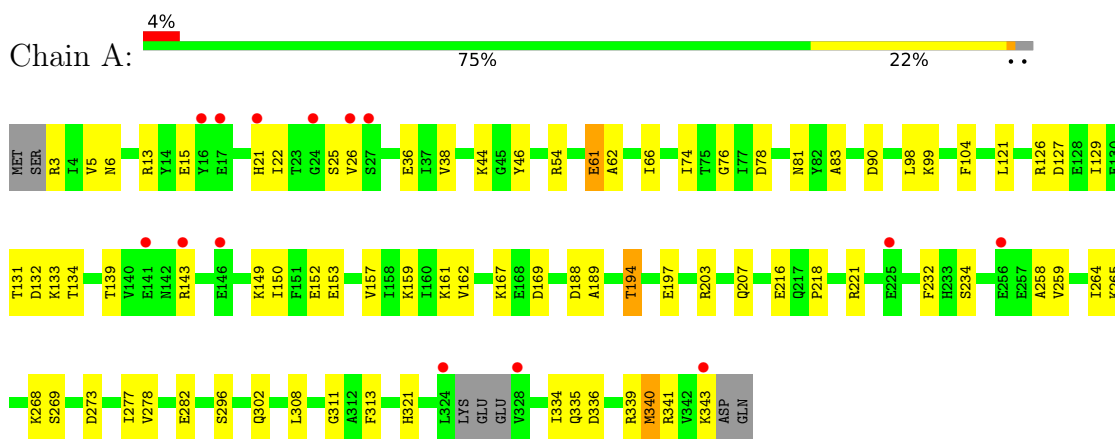
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	52	Total 52	O 52	0	0
3	E	63	Total 63	O 63	0	0
3	F	63	Total 63	O 63	0	0
3	G	65	Total 65	O 65	0	0
3	H	78	Total 78	O 78	0	0
3	I	77	Total 77	O 77	0	0
3	J	75	Total 75	O 75	0	0
3	K	56	Total 56	O 56	0	0
3	L	59	Total 59	O 59	0	0
3	M	67	Total 67	O 67	0	0
3	N	65	Total 65	O 65	0	0
3	O	63	Total 63	O 63	0	0
3	P	66	Total 66	O 66	0	0

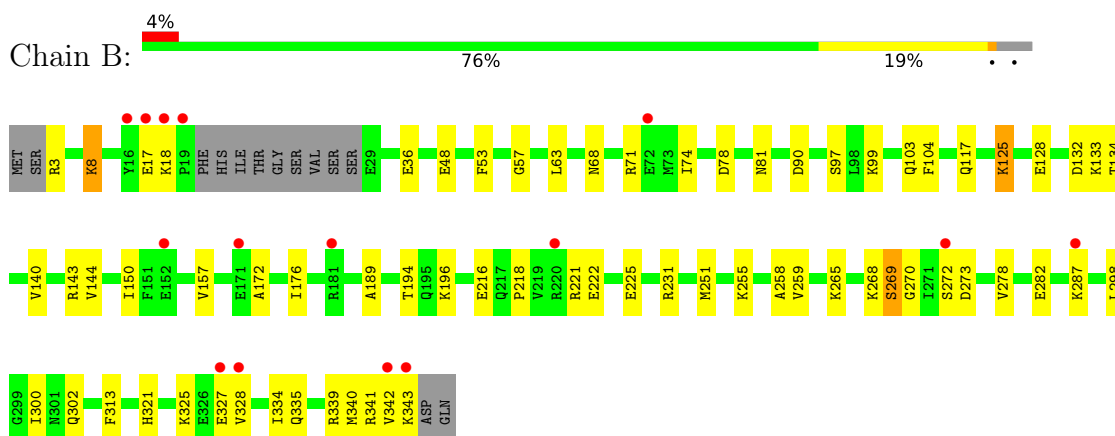
### 3 Residue-property plots [i](#)

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.

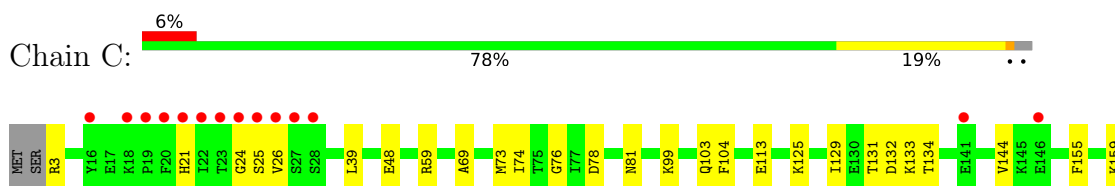
- Molecule 1: Muconate cycloisomerase

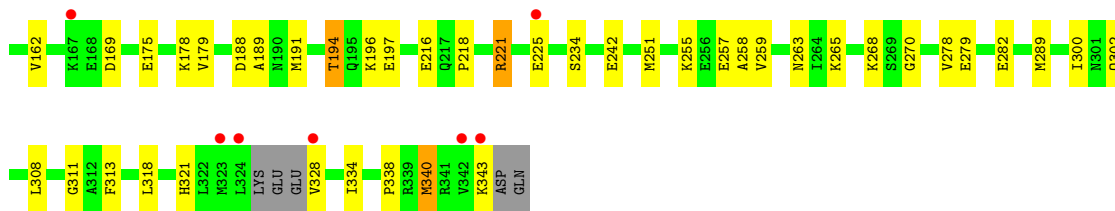


- Molecule 1: Muconate cycloisomerase

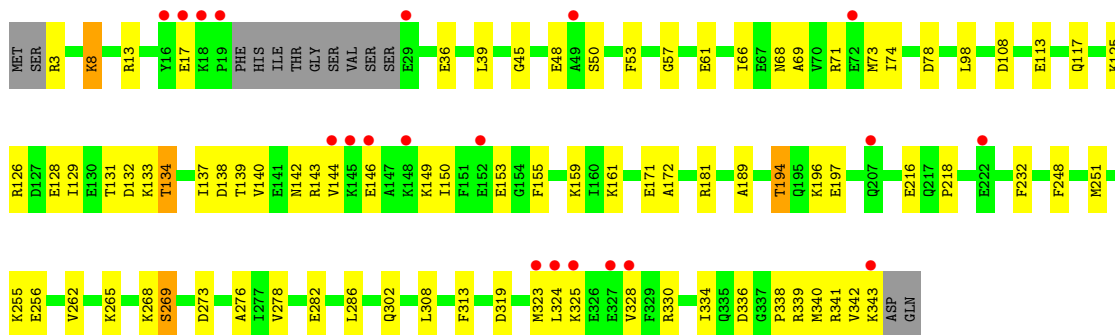
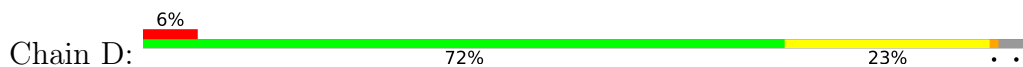


- Molecule 1: Muconate cycloisomerase

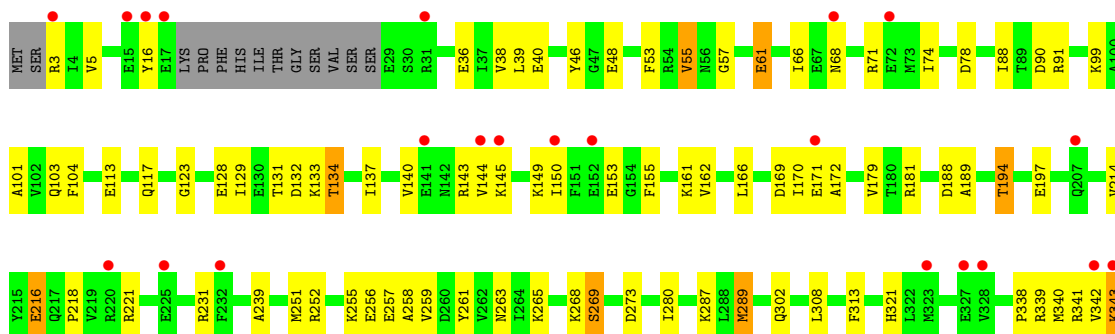




● Molecule 1: Muconate cycloisomerase

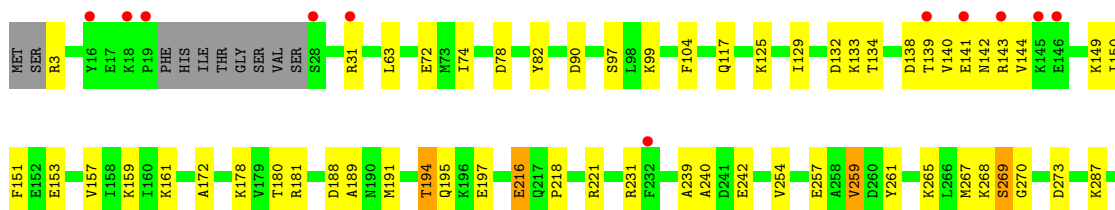
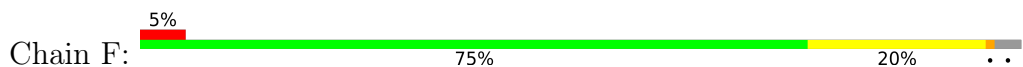


● Molecule 1: Muconate cycloisomerase

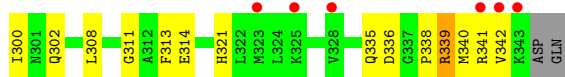


ASP  
GLN

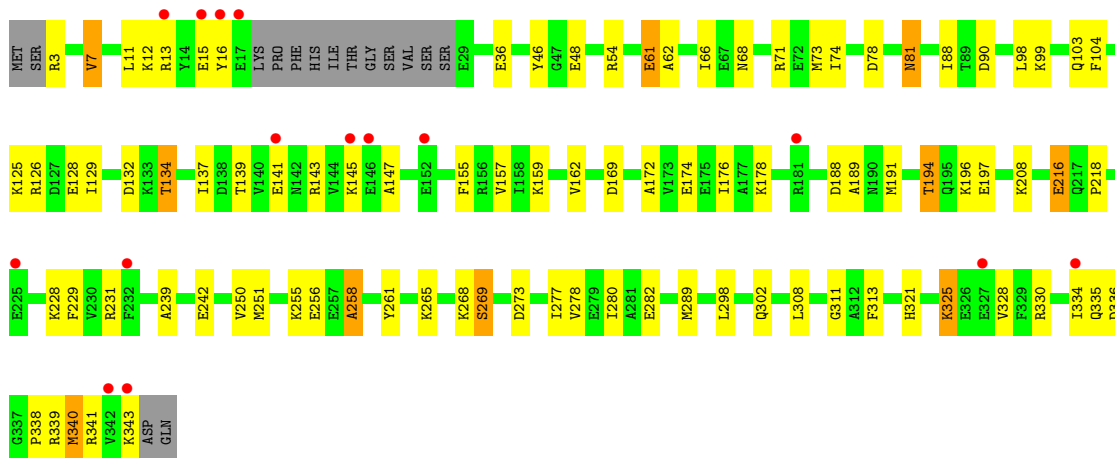
● Molecule 1: Muconate cycloisomerase



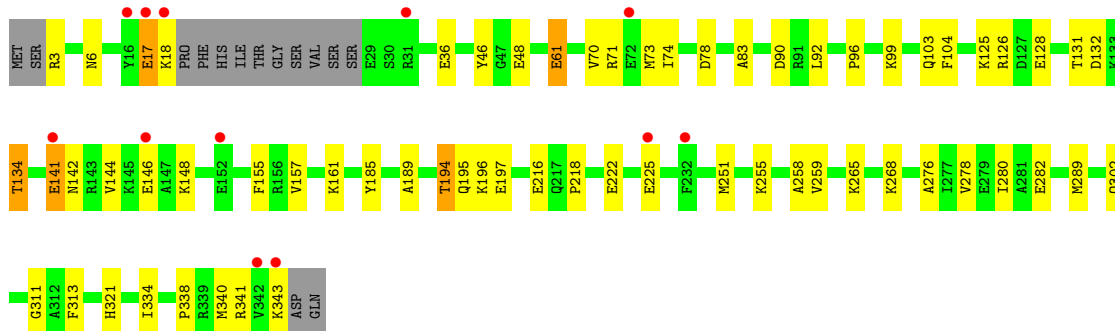
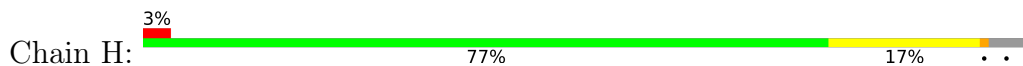
F151  
E152  
E153  
V157  
I158  
K159  
I160  
K161  
A172  
K178  
V179  
T180  
R181  
D188  
A189  
N190  
M191  
T194  
Q195  
K196  
E197  
E216  
Q217  
P218  
R221  
R231  
L98  
K99  
F104  
A239  
A240  
D241  
E242  
V254  
E257  
A258  
V259  
Y261  
K265  
L266  
K267  
K268  
S269  
G270  
D273  
K287



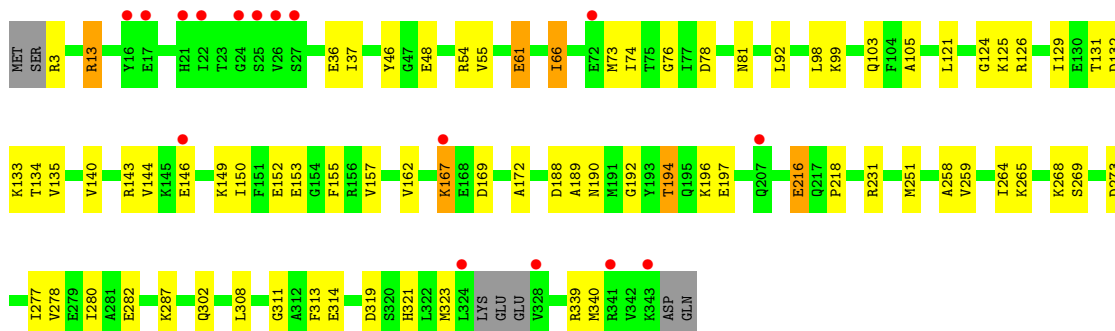
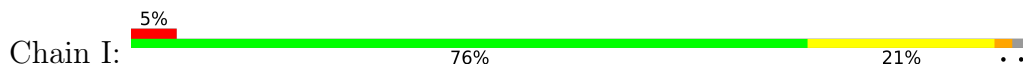
- Molecule 1: Muconate cycloisomerase



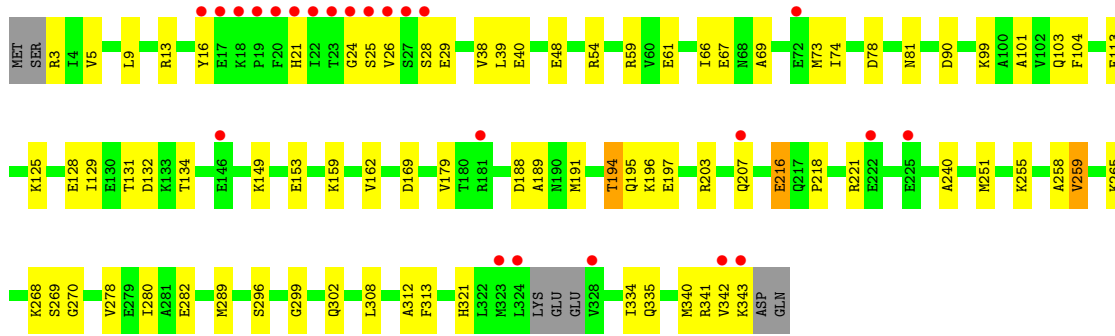
- Molecule 1: Muconate cycloisomerase



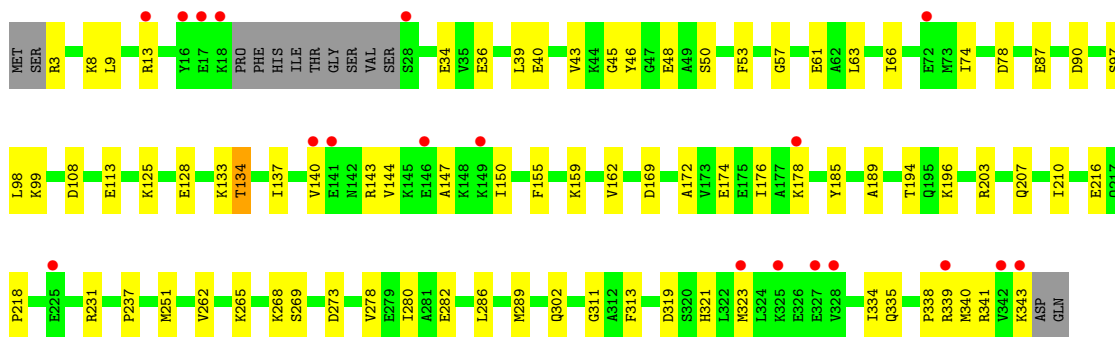
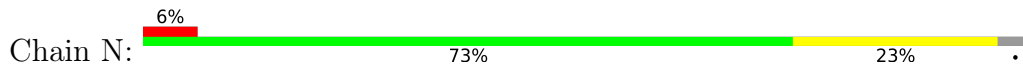
- Molecule 1: Muconate cycloisomerase



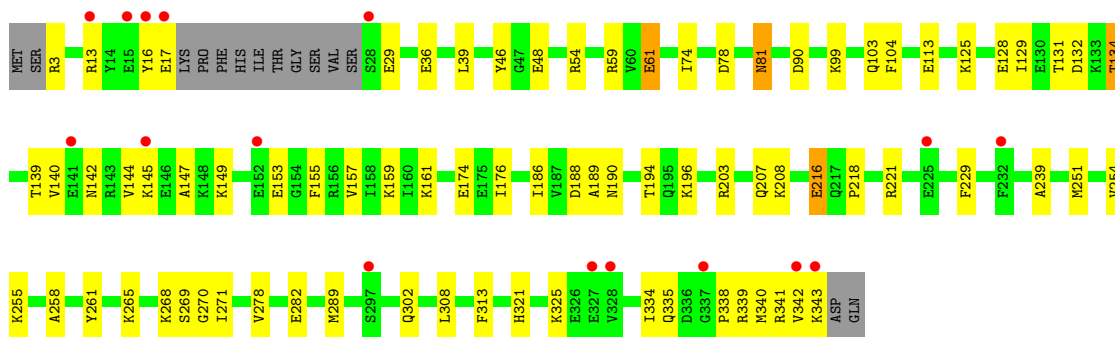
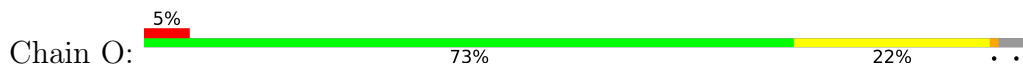




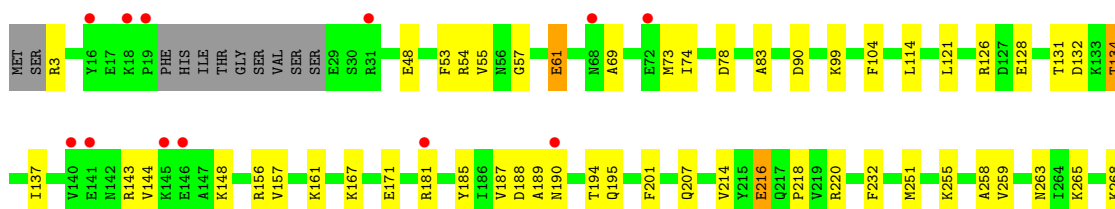
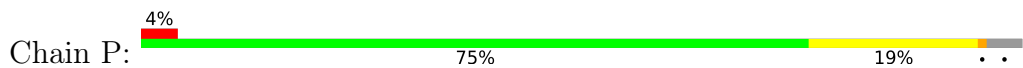
- Molecule 1: Muconate cycloisomerase

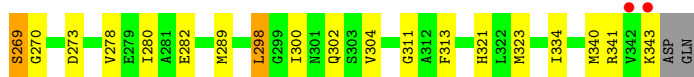


- Molecule 1: Muconate cycloisomerase



- Molecule 1: Muconate cycloisomerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.81Å 165.14Å 209.64Å 90.00° 96.06° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 25.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.00-2.10) 98.9 (25.00-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 1.88Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.246 , 0.277 0.246 , 0.275	Depositor DCC
$R_{free}$ test set	26792 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtrriage
Anisotropy	0.778	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.58$ , $\langle L^2 \rangle = 0.42$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	43115	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5515e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [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	0.41	0/2698	0.93	10/3624 (0.3%)
1	B	0.38	0/2658	0.92	10/3568 (0.3%)
1	C	0.38	0/2698	0.93	10/3624 (0.3%)
1	D	0.38	0/2658	0.92	8/3568 (0.2%)
1	E	0.39	0/2641	0.92	10/3545 (0.3%)
1	F	0.38	0/2664	0.92	8/3576 (0.2%)
1	G	0.40	0/2641	0.92	9/3545 (0.3%)
1	H	0.39	0/2650	0.94	10/3556 (0.3%)
1	I	0.40	0/2698	0.94	11/3624 (0.3%)
1	J	0.40	0/2650	0.93	11/3556 (0.3%)
1	K	0.38	0/2641	0.93	9/3545 (0.3%)
1	L	0.38	0/2647	0.93	9/3553 (0.3%)
1	M	0.39	0/2698	0.95	16/3624 (0.4%)
1	N	0.39	0/2656	0.91	9/3564 (0.3%)
1	O	0.39	0/2647	0.92	10/3553 (0.3%)
1	P	0.39	0/2658	0.93	11/3568 (0.3%)
All	All	0.39	0/42603	0.93	161/57193 (0.3%)

There are no bond length outliers.

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	194	THR	N-CA-C	-8.81	98.65	110.55
1	E	194	THR	N-CA-C	-8.32	99.80	110.53
1	H	194	THR	N-CA-C	-7.57	100.77	110.53
1	M	194	THR	N-CA-C	-7.41	100.98	110.53
1	C	194	THR	N-CA-C	-7.35	101.05	110.53

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	2660	0	2697	46	0
1	B	2622	0	2661	46	0
1	C	2660	0	2697	47	0
1	D	2622	0	2661	62	0
1	E	2606	0	2641	61	0
1	F	2628	0	2666	46	0
1	G	2606	0	2641	70	0
1	H	2615	0	2654	42	0
1	I	2660	0	2697	54	0
1	J	2615	0	2654	50	0
1	K	2606	0	2641	64	0
1	L	2612	0	2646	40	0
1	M	2660	0	2697	46	0
1	N	2621	0	2659	47	0
1	O	2612	0	2646	54	0
1	P	2622	0	2661	49	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
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	83	0	0	2	0
3	B	73	0	0	1	0
3	C	67	0	0	1	0
3	D	52	0	0	0	0
3	E	63	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	63	0	0	1	0
3	G	65	0	0	0	0
3	H	78	0	0	1	0
3	I	77	0	0	4	0
3	J	75	0	0	0	0
3	K	56	0	0	1	0
3	L	59	0	0	1	0
3	M	67	0	0	0	0
3	N	65	0	0	0	0
3	O	63	0	0	0	0
3	P	66	0	0	2	0
All	All	43115	0	42619	789	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 9.

The worst 5 of 789 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:C:191:MET:HE3	1:C:221:ARG:H	1.09	1.14
1:O:334:ILE:HD11	1:O:343:LYS:HG2	1.50	0.92
1:A:131:THR:HG22	1:A:340:MET:HE1	1.52	0.90
1:C:191:MET:HE3	1:C:221:ARG:N	1.87	0.89
1:I:73:MET:HE1	1:I:92:LEU:HD21	1.55	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	334/345 (97%)	320 (96%)	14 (4%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	328/345 (95%)	316 (96%)	12 (4%)	0	100	100
1	C	334/345 (97%)	320 (96%)	14 (4%)	0	100	100
1	D	328/345 (95%)	314 (96%)	14 (4%)	0	100	100
1	E	326/345 (94%)	312 (96%)	13 (4%)	1 (0%)	36	36
1	F	329/345 (95%)	315 (96%)	14 (4%)	0	100	100
1	G	326/345 (94%)	316 (97%)	10 (3%)	0	100	100
1	H	327/345 (95%)	315 (96%)	12 (4%)	0	100	100
1	I	334/345 (97%)	320 (96%)	14 (4%)	0	100	100
1	J	327/345 (95%)	314 (96%)	13 (4%)	0	100	100
1	K	326/345 (94%)	310 (95%)	16 (5%)	0	100	100
1	L	327/345 (95%)	315 (96%)	12 (4%)	0	100	100
1	M	334/345 (97%)	321 (96%)	13 (4%)	0	100	100
1	N	328/345 (95%)	312 (95%)	16 (5%)	0	100	100
1	O	327/345 (95%)	315 (96%)	12 (4%)	0	100	100
1	P	328/345 (95%)	316 (96%)	12 (4%)	0	100	100
All	All	5263/5520 (95%)	5051 (96%)	211 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	16	TYR

### 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	285/292 (98%)	281 (99%)	4 (1%)	59	67
1	B	280/292 (96%)	274 (98%)	6 (2%)	47	54
1	C	285/292 (98%)	284 (100%)	1 (0%)	84	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	280/292 (96%)	276 (99%)	4 (1%)	59	67
1	E	278/292 (95%)	276 (99%)	2 (1%)	76	83
1	F	281/292 (96%)	278 (99%)	3 (1%)	65	74
1	G	278/292 (95%)	273 (98%)	5 (2%)	51	60
1	H	279/292 (96%)	276 (99%)	3 (1%)	65	74
1	I	285/292 (98%)	281 (99%)	4 (1%)	59	67
1	J	279/292 (96%)	277 (99%)	2 (1%)	76	83
1	K	278/292 (95%)	272 (98%)	6 (2%)	45	53
1	L	279/292 (96%)	275 (99%)	4 (1%)	59	67
1	M	285/292 (98%)	285 (100%)	0	100	100
1	N	280/292 (96%)	278 (99%)	2 (1%)	76	83
1	O	279/292 (96%)	278 (100%)	1 (0%)	84	89
1	P	280/292 (96%)	276 (99%)	4 (1%)	59	67
All	All	4491/4672 (96%)	4440 (99%)	51 (1%)	65	74

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	13	ARG
1	K	29	GLU
1	P	298	LEU
1	I	61	GLU
1	J	13	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	233	HIS
1	N	142	ASN
1	K	335	GLN
1	M	6	ASN
1	O	56	ASN

### 5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	338/345 (97%)	0.09	14 (4%) 41 43	18, 28, 47, 58	0
1	B	332/345 (96%)	0.24	15 (4%) 38 40	20, 29, 51, 66	0
1	C	338/345 (97%)	0.35	21 (6%) 26 28	19, 30, 52, 62	0
1	D	332/345 (96%)	0.48	20 (6%) 27 29	22, 33, 54, 67	0
1	E	330/345 (95%)	0.39	22 (6%) 24 25	21, 31, 51, 65	0
1	F	333/345 (96%)	0.38	17 (5%) 33 35	20, 32, 52, 66	0
1	G	330/345 (95%)	0.34	15 (4%) 38 40	19, 30, 49, 65	0
1	H	331/345 (95%)	0.21	12 (3%) 46 48	18, 28, 47, 65	0
1	I	338/345 (97%)	0.15	16 (4%) 36 38	18, 27, 48, 58	0
1	J	331/345 (95%)	0.26	20 (6%) 27 29	19, 29, 50, 64	0
1	K	330/345 (95%)	0.43	17 (5%) 33 35	22, 32, 51, 65	0
1	L	331/345 (95%)	0.33	13 (3%) 43 45	22, 33, 52, 64	0
1	M	338/345 (97%)	0.39	24 (7%) 22 23	20, 30, 53, 64	0
1	N	332/345 (96%)	0.44	19 (5%) 29 31	21, 31, 53, 66	0
1	O	331/345 (95%)	0.26	16 (4%) 35 38	18, 30, 49, 63	0
1	P	332/345 (96%)	0.25	14 (4%) 40 42	18, 30, 49, 65	0
All	All	5327/5520 (96%)	0.31	275 (5%) 33 35	18, 30, 51, 67	0

The worst 5 of 275 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	19	PRO	7.0
1	M	324	LEU	6.4
1	D	19	PRO	5.3
1	C	324	LEU	5.0
1	C	24	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 oligosaccharides 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
2	MG	J	401	1/1	0.87	0.08	27,27,27,27	0
2	MG	C	401	1/1	0.91	0.07	24,24,24,24	0
2	MG	I	401	1/1	0.91	0.06	26,26,26,26	0
2	MG	A	401	1/1	0.91	0.08	26,26,26,26	0
2	MG	O	401	1/1	0.91	0.07	27,27,27,27	0
2	MG	M	401	1/1	0.92	0.07	27,27,27,27	0
2	MG	B	401	1/1	0.93	0.05	27,27,27,27	0
2	MG	F	401	1/1	0.93	0.05	29,29,29,29	0
2	MG	L	401	1/1	0.94	0.06	29,29,29,29	0
2	MG	D	401	1/1	0.94	0.05	28,28,28,28	0
2	MG	H	401	1/1	0.94	0.06	25,25,25,25	0
2	MG	G	401	1/1	0.95	0.05	26,26,26,26	0
2	MG	P	401	1/1	0.95	0.06	25,25,25,25	0
2	MG	N	401	1/1	0.96	0.05	29,29,29,29	0
2	MG	K	401	1/1	0.98	0.03	30,30,30,30	0
2	MG	E	401	1/1	0.99	0.02	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.