



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:53 am GMT

PDB ID : 3DFY
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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

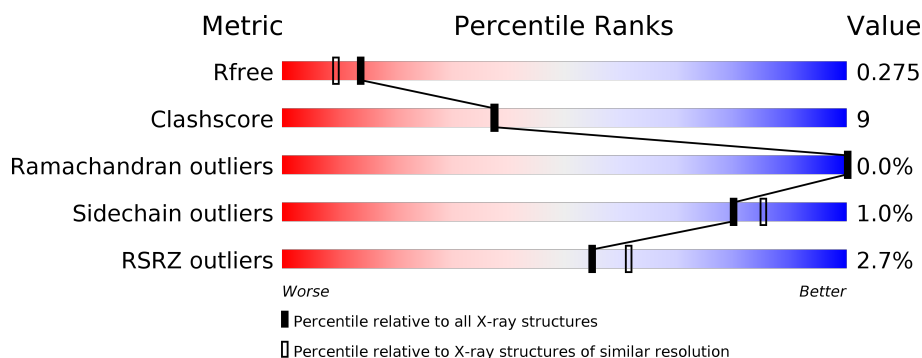
1 Overall quality at a glance

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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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 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 $\leq 5\%$. 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	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>••</div> </div> </div>
1	B	345	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>••</div> </div> </div>
1	C	345	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>•</div> </div> </div>
1	D	345	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>••</div> </div> </div>
1	E	345	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>•</div> </div> </div>
1	F	345	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>•</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	345	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>71%</div><div>24%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	H	345	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>81%</div><div>15%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	I	345	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>79%</div><div>19%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	J	345	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>79%</div><div>16%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	K	345	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>70%</div><div>25%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	L	345	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>78%</div><div>18%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	M	345	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>81%</div><div>17%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	N	345	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>77%</div><div>19%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	O	345	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>75%</div><div>21%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	P	345	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>78%</div><div>18%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>

2 Entry composition

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total 1	Mg 1	0	0
2	G	1	Total 1	Mg 1	0	0
2	J	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	K	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0
2	H	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	I	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	N	1	Total 1	Mg 1	0	0
2	O	1	Total 1	Mg 1	0	0
2	L	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0
2	M	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

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

Continued on next page...

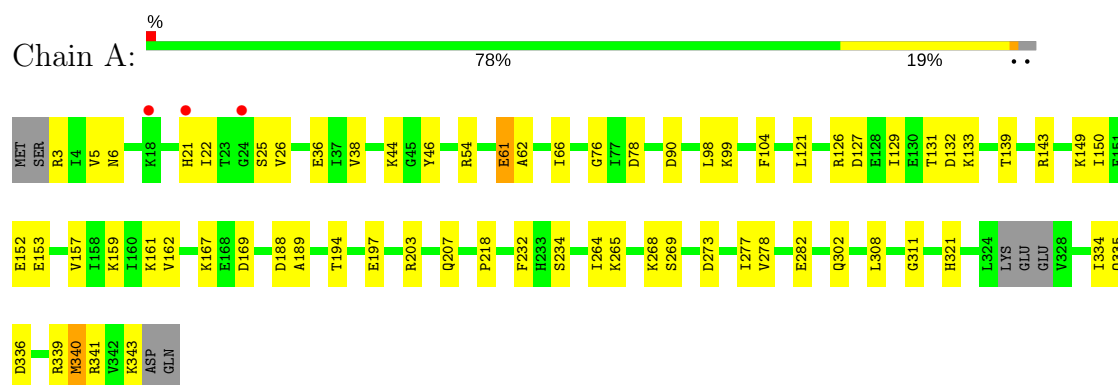
Continued from previous page...

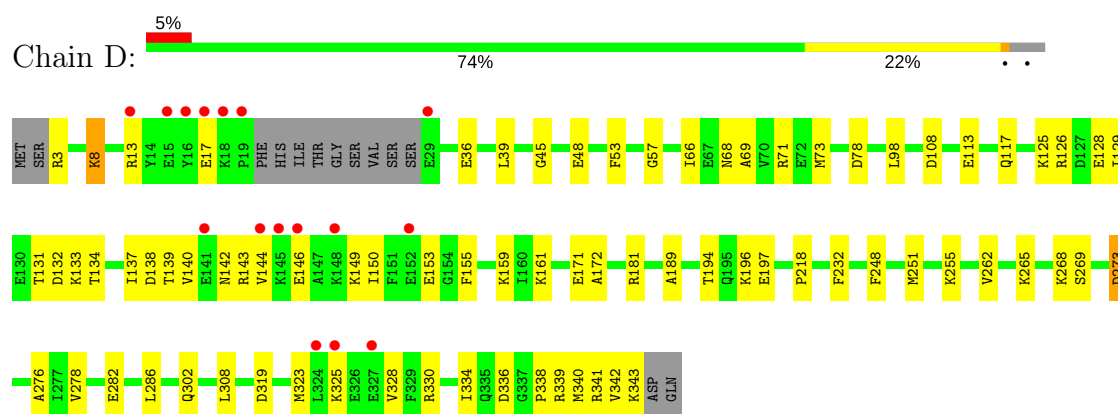
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	52	Total 52	O 52	0	0
3	E	63	Total 63	O 63	0	0
3	F	63	Total 63	O 63	0	0
3	G	65	Total 65	O 65	0	0
3	H	78	Total 78	O 78	0	0
3	I	77	Total 77	O 77	0	0
3	J	75	Total 75	O 75	0	0
3	K	56	Total 56	O 56	0	0
3	L	59	Total 59	O 59	0	0
3	M	67	Total 67	O 67	0	0
3	N	65	Total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

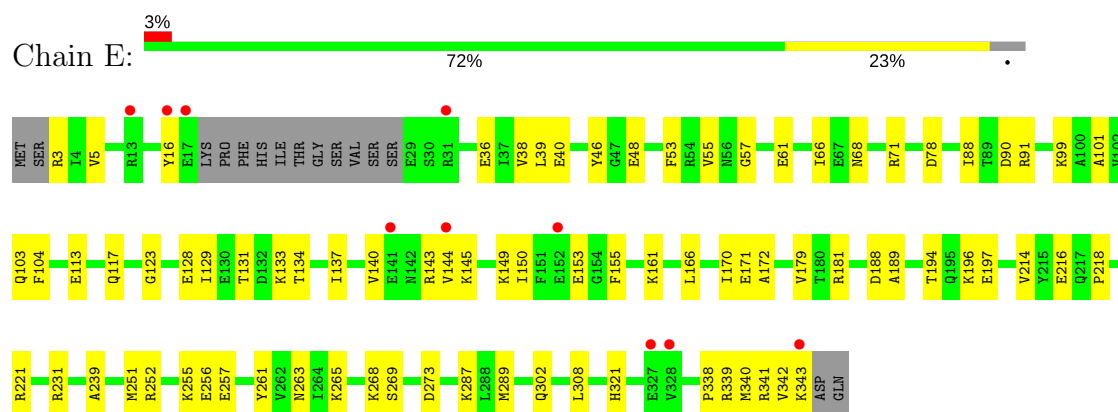
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Muconate cycloisomerase

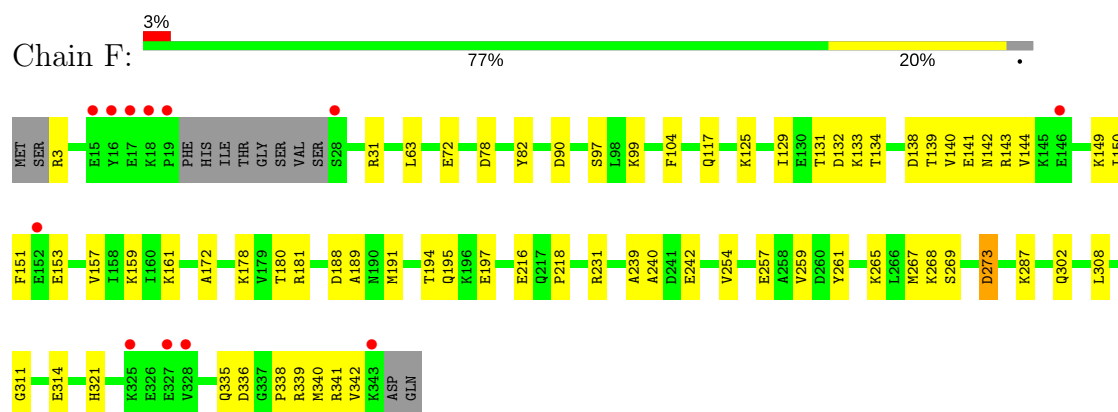




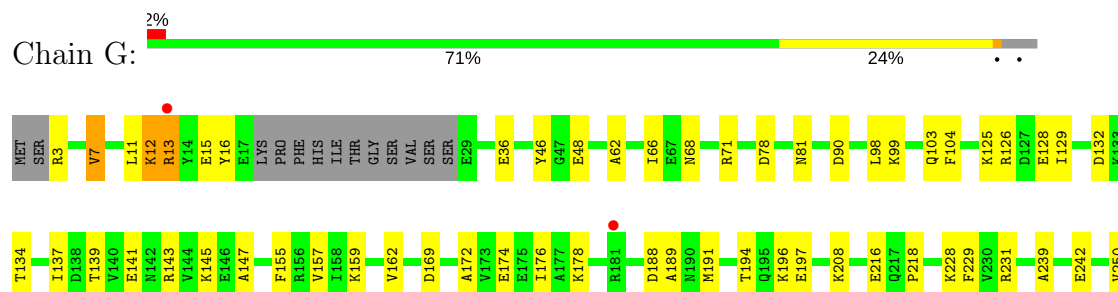
• Molecule 1: Muconate cycloisomerase



• Molecule 1: Muconate cycloisomerase

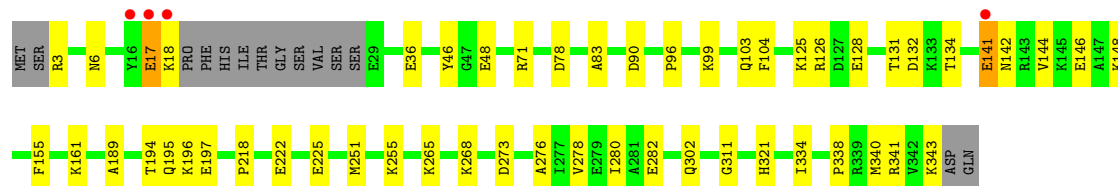
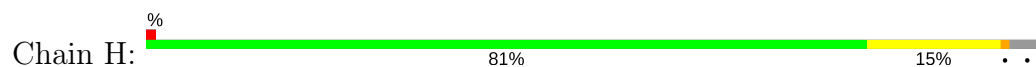


• Molecule 1: Muconate cycloisomerase

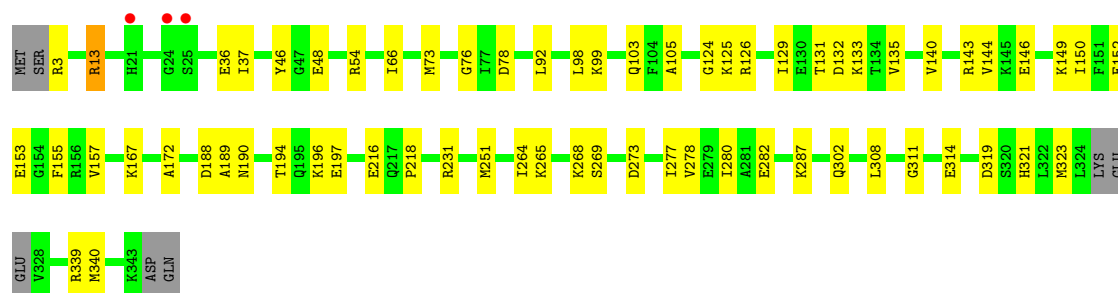




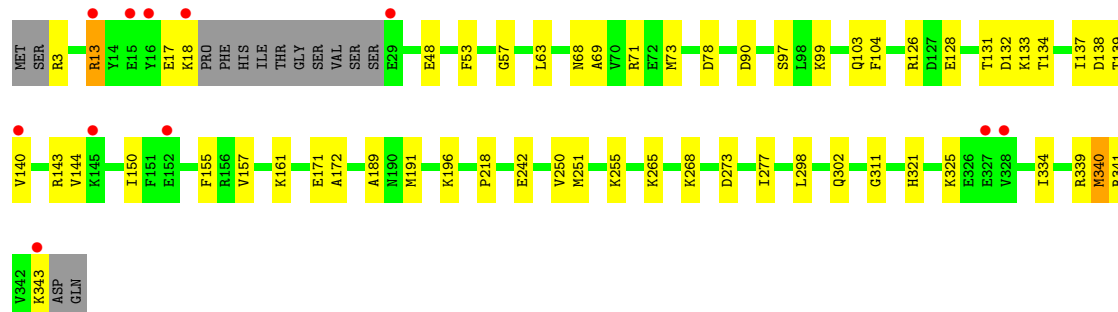
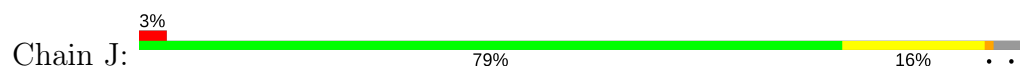
- Molecule 1: Muconate cycloisomerase



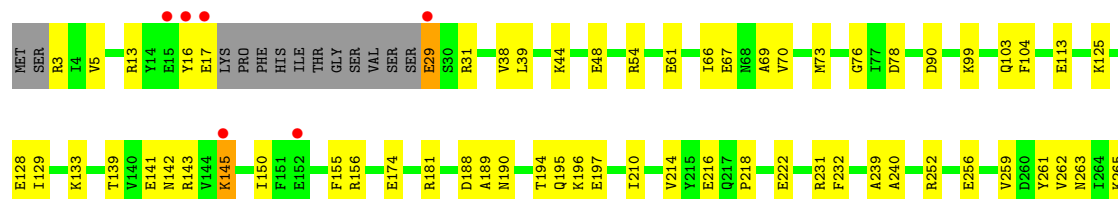
- Molecule 1: Muconate cycloisomerase



- Molecule 1: Muconate cycloisomerase

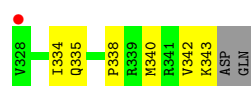
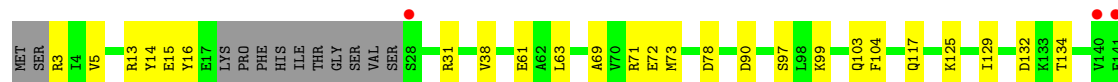
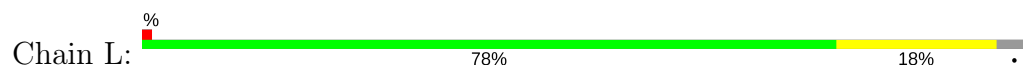


- Molecule 1: Muconate cycloisomerase

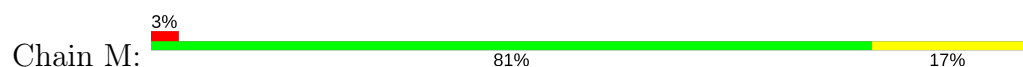




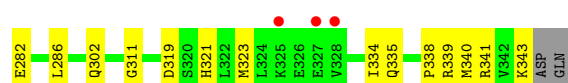
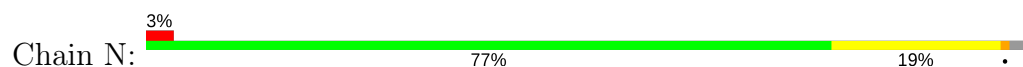
• Molecule 1: Muconate cycloisomerase



• Molecule 1: Muconate cycloisomerase

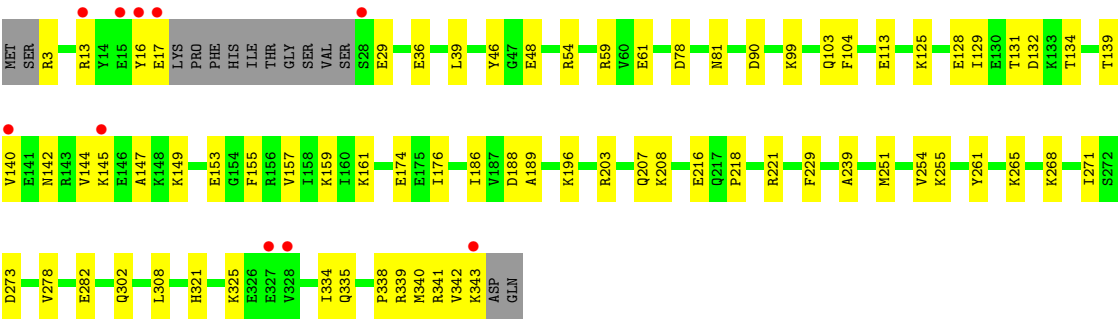


• Molecule 1: Muconate cycloisomerase

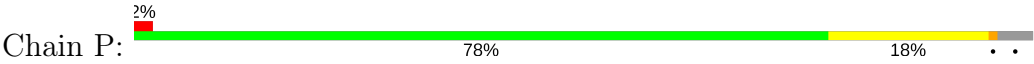


• Molecule 1: Muconate cycloisomerase





● Molecule 1: Muconate cycloisomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.81Å 165.14Å 209.64Å 90.00° 96.06° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 39.73 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.00-2.10) 93.9 (39.73-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	20322 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	25.7	Xtrriage
Anisotropy	0.778	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.42$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.35	0/2698	0.62	0/3624
1	B	0.34	0/2658	0.61	0/3568
1	C	0.34	0/2698	0.62	0/3624
1	D	0.33	0/2658	0.60	0/3568
1	E	0.35	0/2641	0.61	0/3545
1	F	0.34	0/2664	0.60	0/3576
1	G	0.35	0/2641	0.61	0/3545
1	H	0.35	0/2650	0.62	0/3556
1	I	0.35	0/2698	0.62	0/3624
1	J	0.35	0/2650	0.61	0/3556
1	K	0.34	0/2641	0.61	0/3545
1	L	0.32	0/2647	0.60	0/3553
1	M	0.33	0/2698	0.62	0/3624
1	N	0.34	0/2656	0.61	0/3564
1	O	0.34	0/2647	0.61	0/3553
1	P	0.34	0/2658	0.61	0/3568
All	All	0.34	0/42603	0.61	0/57193

There are no bond length outliers.

There are no bond angle outliers.

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	2660	0	2697	43	0
1	B	2622	0	2661	42	0
1	C	2660	0	2697	48	0
1	D	2622	0	2661	61	0
1	E	2606	0	2641	57	0
1	F	2628	0	2666	46	0
1	G	2606	0	2641	64	0
1	H	2615	0	2654	37	0
1	I	2660	0	2697	50	0
1	J	2615	0	2654	47	0
1	K	2606	0	2641	61	0
1	L	2612	0	2646	37	0
1	M	2660	0	2697	40	0
1	N	2621	0	2659	44	0
1	O	2612	0	2646	53	0
1	P	2622	0	2661	46	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
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	3	0
3	J	75	0	0	0	0
3	K	56	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	742	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 742 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:O:334:ILE:HD11	1:O:343:LYS:HG2	1.50	0.92
1:C:191:MET:HE3	1:C:221:ARG:H	1.37	0.89
1:D:334:ILE:HD11	1:D:343:LYS:HE3	1.59	0.84
1:J:131:THR:HG22	1:J:340:MET:HE1	1.60	0.84
1:G:339:ARG:HB2	1:G:339:ARG:HH11	1.48	0.79

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	100	100
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%)	44	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	71	78
1	B	280/292 (96%)	274 (98%)	6 (2%)	59	64
1	C	285/292 (98%)	283 (99%)	2 (1%)	87	91
1	D	280/292 (96%)	278 (99%)	2 (1%)	87	91
1	E	278/292 (95%)	277 (100%)	1 (0%)	93	95
1	F	281/292 (96%)	279 (99%)	2 (1%)	87	91
1	G	278/292 (95%)	273 (98%)	5 (2%)	64	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	279/292 (96%)	276 (99%)	3 (1%)	78	83
1	I	285/292 (98%)	284 (100%)	1 (0%)	93	95
1	J	279/292 (96%)	276 (99%)	3 (1%)	78	83
1	K	278/292 (95%)	273 (98%)	5 (2%)	64	70
1	L	279/292 (96%)	276 (99%)	3 (1%)	78	83
1	M	285/292 (98%)	285 (100%)	0	100	100
1	N	280/292 (96%)	277 (99%)	3 (1%)	78	83
1	O	279/292 (96%)	278 (100%)	1 (0%)	93	95
1	P	280/292 (96%)	276 (99%)	4 (1%)	71	78
All	All	4491/4672 (96%)	4446 (99%)	45 (1%)	80	85

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	68	ASN
1	I	13	ARG
1	P	207	GLN
1	H	17	GLU
1	J	13	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	81	ASN
1	I	302	GLN
1	P	81	ASN
1	H	142	ASN
1	H	302	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	338/345 (97%)	-0.21	3 (0%) 84 86	18, 28, 47, 58	0
1	B	332/345 (96%)	-0.18	10 (3%) 51 58	20, 29, 51, 66	0
1	C	338/345 (97%)	-0.14	14 (4%) 38 45	19, 30, 52, 62	0
1	D	332/345 (96%)	-0.00	16 (4%) 31 37	22, 33, 54, 67	0
1	E	330/345 (95%)	-0.10	10 (3%) 51 58	21, 31, 51, 65	0
1	F	333/345 (96%)	-0.04	12 (3%) 43 50	20, 32, 52, 66	0
1	G	330/345 (95%)	-0.11	6 (1%) 69 73	19, 30, 49, 65	0
1	H	331/345 (95%)	-0.25	4 (1%) 79 82	18, 28, 47, 65	0
1	I	338/345 (97%)	-0.14	3 (0%) 84 86	18, 27, 48, 58	0
1	J	331/345 (95%)	-0.13	11 (3%) 47 54	19, 29, 50, 64	0
1	K	330/345 (95%)	-0.06	11 (3%) 47 54	22, 32, 51, 65	0
1	L	331/345 (95%)	-0.13	5 (1%) 74 77	22, 33, 52, 64	0
1	M	338/345 (97%)	-0.12	12 (3%) 43 50	20, 30, 53, 64	0
1	N	332/345 (96%)	-0.05	11 (3%) 47 54	21, 31, 53, 66	0
1	O	331/345 (95%)	-0.14	10 (3%) 51 58	18, 30, 49, 63	0
1	P	332/345 (96%)	-0.15	7 (2%) 64 68	18, 30, 49, 65	0
All	All	5327/5520 (96%)	-0.12	145 (2%) 55 61	18, 30, 51, 67	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	19	PRO	8.5
1	F	19	PRO	7.0
1	O	28	SER	6.8
1	F	18	LYS	6.1
1	E	327	GLU	5.3

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
2	MG	C	401	1/1	0.93	0.13	0.96	24,24,24,24	0
2	MG	A	401	1/1	0.81	0.12	0.29	26,26,26,26	0
2	MG	O	401	1/1	0.89	0.10	-0.39	27,27,27,27	0
2	MG	I	401	1/1	0.88	0.10	-0.50	26,26,26,26	0
2	MG	M	401	1/1	0.88	0.11	-0.56	27,27,27,27	0
2	MG	J	401	1/1	0.79	0.10	-0.71	27,27,27,27	0
2	MG	L	401	1/1	0.82	0.09	-0.81	29,29,29,29	0
2	MG	P	401	1/1	0.87	0.09	-0.82	25,25,25,25	0
2	MG	H	401	1/1	0.91	0.08	-1.06	25,25,25,25	0
2	MG	F	401	1/1	0.86	0.09	-1.26	29,29,29,29	0
2	MG	N	401	1/1	0.87	0.07	-1.32	29,29,29,29	0
2	MG	D	401	1/1	0.85	0.07	-1.78	28,28,28,28	0
2	MG	G	401	1/1	0.96	0.08	-1.92	26,26,26,26	0
2	MG	B	401	1/1	0.92	0.07	-2.08	27,27,27,27	0
2	MG	E	401	1/1	0.97	0.06	-2.56	29,29,29,29	0
2	MG	K	401	1/1	0.96	0.06	-3.33	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.