



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:38 PM GMT

PDB ID : 1UJQ  
Title : Crystal structure of 2-methylisocitrate lyase (PrpB) from *Salmonella enterica* serovar typhimurium  
Authors : Simanshu, D.K.; Murthy, M.R.N.  
Deposited on : 2003-08-11  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

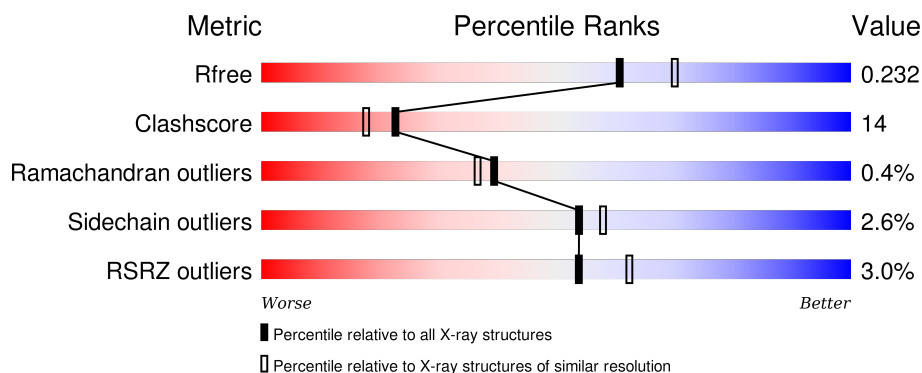
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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  $\geq 3$ , 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	305	<div> <div>3%</div> <div>71% 16% • 11%</div> </div>
1	B	305	<div> <div>%</div> <div>73% 13% • 12%</div> </div>
1	C	305	<div> <div>3%</div> <div>63% 26% • 10%</div> </div>
1	D	305	<div> <div>5%</div> <div>62% 25% • 12%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8785 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 Probable methylisocitrate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	1	0
			2068	1303	358	399	8			
1	B	268	Total	C	N	O	S	0	1	0
			2038	1284	353	393	8			
1	C	275	Total	C	N	O	S	0	0	0
			2087	1316	362	401	8			
1	D	268	Total	C	N	O	S	0	0	0
			2027	1279	354	386	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	CLONING ARTIFACT	UNP Q56062
A	0	ALA	-	CLONING ARTIFACT	UNP Q56062
A	1	SER	-	CLONING ARTIFACT	UNP Q56062
A	296	LEU	-	EXPRESSION TAG	UNP Q56062
A	297	GLU	-	EXPRESSION TAG	UNP Q56062
A	298	HIS	-	EXPRESSION TAG	UNP Q56062
A	299	HIS	-	EXPRESSION TAG	UNP Q56062
A	300	HIS	-	EXPRESSION TAG	UNP Q56062
A	301	HIS	-	EXPRESSION TAG	UNP Q56062
A	302	HIS	-	EXPRESSION TAG	UNP Q56062
A	303	HIS	-	EXPRESSION TAG	UNP Q56062
B	-1	MET	-	CLONING ARTIFACT	UNP Q56062
B	0	ALA	-	CLONING ARTIFACT	UNP Q56062
B	1	SER	-	CLONING ARTIFACT	UNP Q56062
B	296	LEU	-	EXPRESSION TAG	UNP Q56062
B	297	GLU	-	EXPRESSION TAG	UNP Q56062
B	298	HIS	-	EXPRESSION TAG	UNP Q56062
B	299	HIS	-	EXPRESSION TAG	UNP Q56062
B	300	HIS	-	EXPRESSION TAG	UNP Q56062
B	301	HIS	-	EXPRESSION TAG	UNP Q56062
B	302	HIS	-	EXPRESSION TAG	UNP Q56062

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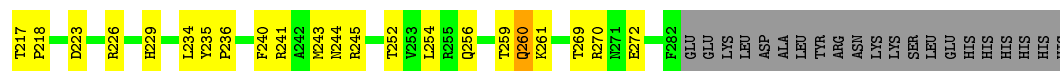
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Chain	Residue	Modelled	Actual	Comment	Reference
B	303	HIS	-	EXPRESSION TAG	UNP Q56062
C	-1	MET	-	CLONING ARTIFACT	UNP Q56062
C	0	ALA	-	CLONING ARTIFACT	UNP Q56062
C	1	SER	-	CLONING ARTIFACT	UNP Q56062
C	296	LEU	-	EXPRESSION TAG	UNP Q56062
C	297	GLU	-	EXPRESSION TAG	UNP Q56062
C	298	HIS	-	EXPRESSION TAG	UNP Q56062
C	299	HIS	-	EXPRESSION TAG	UNP Q56062
C	300	HIS	-	EXPRESSION TAG	UNP Q56062
C	301	HIS	-	EXPRESSION TAG	UNP Q56062
C	302	HIS	-	EXPRESSION TAG	UNP Q56062
C	303	HIS	-	EXPRESSION TAG	UNP Q56062
D	-1	MET	-	CLONING ARTIFACT	UNP Q56062
D	0	ALA	-	CLONING ARTIFACT	UNP Q56062
D	1	SER	-	CLONING ARTIFACT	UNP Q56062
D	296	LEU	-	EXPRESSION TAG	UNP Q56062
D	297	GLU	-	EXPRESSION TAG	UNP Q56062
D	298	HIS	-	EXPRESSION TAG	UNP Q56062
D	299	HIS	-	EXPRESSION TAG	UNP Q56062
D	300	HIS	-	EXPRESSION TAG	UNP Q56062
D	301	HIS	-	EXPRESSION TAG	UNP Q56062
D	302	HIS	-	EXPRESSION TAG	UNP Q56062
D	303	HIS	-	EXPRESSION TAG	UNP Q56062

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	179	Total O 179 179	0	0
2	B	175	Total O 175 175	0	0
2	C	121	Total O 121 121	0	0
2	D	90	Total O 90 90	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.81Å 99.09Å 201.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.10 55.61 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.9 (19.99-2.10) 92.9 (55.61-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.84 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.232 0.204 , 0.232	Depositor DCC
$R_{free}$ test set	3514 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 69060 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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	0.30	0/2098	0.56	0/2848
1	B	0.32	0/2068	0.57	0/2809
1	C	0.29	0/2118	0.52	0/2876
1	D	0.27	0/2058	0.52	0/2795
All	All	0.30	0/8342	0.55	0/11328

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	2068	0	2066	46	0
1	B	2038	0	2035	36	0
1	C	2087	0	2089	88	0
1	D	2027	0	2030	74	0
2	A	179	0	0	3	0
2	B	175	0	0	4	0
2	C	121	0	0	5	0
2	D	90	0	0	4	0
All	All	8785	0	8220	223	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 14.



The worst 5 of 223 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:260:GLN:HE21	1:A:260:GLN:H	1.09	0.97
1:C:260:GLN:H	1:C:260:GLN:HE21	0.98	0.96
1:B:260:GLN:HE21	1:B:260:GLN:H	0.98	0.94
1:C:260:GLN:HE21	1:C:260:GLN:N	1.66	0.93
1:D:260:GLN:N	1:D:260:GLN:HE21	1.67	0.92

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	269/305 (88%)	260 (97%)	7 (3%)	2 (1%)	26	21
1	B	265/305 (87%)	262 (99%)	3 (1%)	0	100	100
1	C	271/305 (89%)	259 (96%)	12 (4%)	0	100	100
1	D	264/305 (87%)	259 (98%)	3 (1%)	2 (1%)	24	17
All	All	1069/1220 (88%)	1040 (97%)	25 (2%)	4 (0%)	39	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	90	PHE
1	A	90	PHE
1	A	92	SER
1	D	92	SER

### 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	211/239 (88%)	205 (97%)	6 (3%)	51	55
1	B	208/239 (87%)	201 (97%)	7 (3%)	44	45
1	C	213/239 (89%)	208 (98%)	5 (2%)	58	62
1	D	206/239 (86%)	202 (98%)	4 (2%)	65	70
All	All	838/956 (88%)	816 (97%)	22 (3%)	54	58

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	186	PHE
1	B	260	GLN
1	D	186	PHE
1	B	245	ARG
1	B	254	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	96	ASN
1	C	229	HIS
1	D	256	GLN
1	C	175	GLN
1	C	244	ASN

### 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](#)

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, 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	272/305 (89%)	0.09	8 (2%) 55 63	21, 32, 57, 74	0
1	B	268/305 (87%)	-0.00	2 (0%) 89 91	21, 29, 43, 70	0
1	C	275/305 (90%)	0.21	8 (2%) 55 63	25, 40, 62, 79	0
1	D	268/305 (87%)	0.35	15 (5%) 28 36	25, 45, 68, 93	0
All	All	1083/1220 (88%)	0.16	33 (3%) 54 62	21, 36, 62, 93	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	GLY	5.2
1	B	118	VAL	4.7
1	D	161	ALA	4.4
1	D	88	ILE	4.3
1	D	90	PHE	3.8

### 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.