



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 02:40 PM GMT

PDB ID : 3VBA  
Title : Crystal structure of methanogen 3-isopropylmalate isomerase small subunit  
Authors : Hwang, K.Y.; Lee, E.H.  
Deposited on : 2012-01-02  
Resolution : 2.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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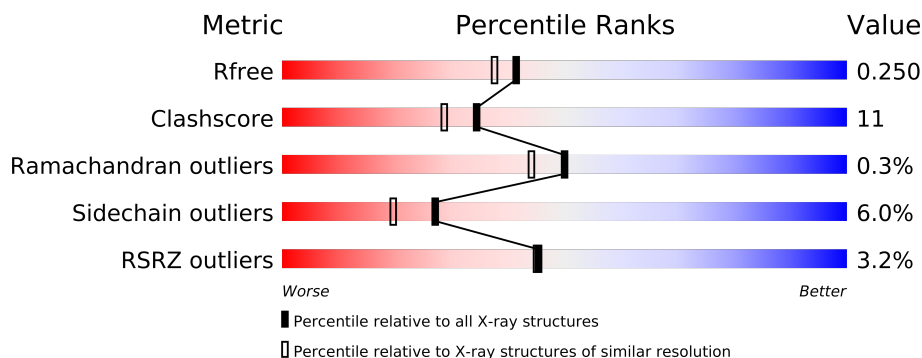
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	176	
1	B	176	
1	C	176	
1	D	176	
1	E	176	
1	F	176	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8356 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Isopropylmalate/citramalate isomerase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1295	828	217	241	9			
1	B	169	Total	C	N	O	S	0	0	0
			1295	828	217	241	9			
1	C	166	Total	C	N	O	S	0	0	0
			1269	812	213	236	8			
1	D	163	Total	C	N	O	S	0	0	0
			1250	801	210	231	8			
1	E	165	Total	C	N	O	S	0	0	0
			1263	809	212	233	9			
1	F	165	Total	C	N	O	S	0	0	0
			1263	809	212	233	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	LEU	-	EXPRESSION TAG	UNP Q58673
A	170	GLU	-	EXPRESSION TAG	UNP Q58673
A	171	HIS	-	EXPRESSION TAG	UNP Q58673
A	172	HIS	-	EXPRESSION TAG	UNP Q58673
A	173	HIS	-	EXPRESSION TAG	UNP Q58673
A	174	HIS	-	EXPRESSION TAG	UNP Q58673
A	175	HIS	-	EXPRESSION TAG	UNP Q58673
A	176	HIS	-	EXPRESSION TAG	UNP Q58673
B	169	LEU	-	EXPRESSION TAG	UNP Q58673
B	170	GLU	-	EXPRESSION TAG	UNP Q58673
B	171	HIS	-	EXPRESSION TAG	UNP Q58673
B	172	HIS	-	EXPRESSION TAG	UNP Q58673
B	173	HIS	-	EXPRESSION TAG	UNP Q58673
B	174	HIS	-	EXPRESSION TAG	UNP Q58673
B	175	HIS	-	EXPRESSION TAG	UNP Q58673
B	176	HIS	-	EXPRESSION TAG	UNP Q58673
C	169	LEU	-	EXPRESSION TAG	UNP Q58673

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Chain	Residue	Modelled	Actual	Comment	Reference
C	170	GLU	-	EXPRESSION TAG	UNP Q58673
C	171	HIS	-	EXPRESSION TAG	UNP Q58673
C	172	HIS	-	EXPRESSION TAG	UNP Q58673
C	173	HIS	-	EXPRESSION TAG	UNP Q58673
C	174	HIS	-	EXPRESSION TAG	UNP Q58673
C	175	HIS	-	EXPRESSION TAG	UNP Q58673
C	176	HIS	-	EXPRESSION TAG	UNP Q58673
D	169	LEU	-	EXPRESSION TAG	UNP Q58673
D	170	GLU	-	EXPRESSION TAG	UNP Q58673
D	171	HIS	-	EXPRESSION TAG	UNP Q58673
D	172	HIS	-	EXPRESSION TAG	UNP Q58673
D	173	HIS	-	EXPRESSION TAG	UNP Q58673
D	174	HIS	-	EXPRESSION TAG	UNP Q58673
D	175	HIS	-	EXPRESSION TAG	UNP Q58673
D	176	HIS	-	EXPRESSION TAG	UNP Q58673
E	169	LEU	-	EXPRESSION TAG	UNP Q58673
E	170	GLU	-	EXPRESSION TAG	UNP Q58673
E	171	HIS	-	EXPRESSION TAG	UNP Q58673
E	172	HIS	-	EXPRESSION TAG	UNP Q58673
E	173	HIS	-	EXPRESSION TAG	UNP Q58673
E	174	HIS	-	EXPRESSION TAG	UNP Q58673
E	175	HIS	-	EXPRESSION TAG	UNP Q58673
E	176	HIS	-	EXPRESSION TAG	UNP Q58673
F	169	LEU	-	EXPRESSION TAG	UNP Q58673
F	170	GLU	-	EXPRESSION TAG	UNP Q58673
F	171	HIS	-	EXPRESSION TAG	UNP Q58673
F	172	HIS	-	EXPRESSION TAG	UNP Q58673
F	173	HIS	-	EXPRESSION TAG	UNP Q58673
F	174	HIS	-	EXPRESSION TAG	UNP Q58673
F	175	HIS	-	EXPRESSION TAG	UNP Q58673
F	176	HIS	-	EXPRESSION TAG	UNP Q58673

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	140	Total O 140 140	0	0
2	B	122	Total O 122 122	0	0
2	C	117	Total O 117 117	0	0
2	D	125	Total O 125 125	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	105	Total 105	O 105	0	0
2	F	112	Total 112	O 112	0	0



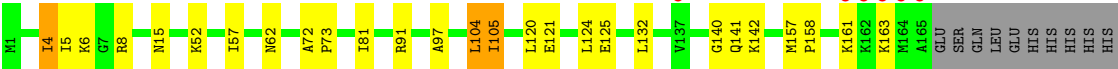
Chain E: 



HIS  
HIS

- Molecule 1: Isopropylmalate/citramalateisomerase small subunit

Chain F: 



HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	33.84Å 107.14Å 288.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.90 – 2.00 43.90 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.90-2.00) 99.0 (43.90-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 1.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.197 , 0.244 0.209 , 0.250	Depositor DCC
$R_{free}$ test set	4871 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 36.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	9 of 97735 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8356	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.86 % 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 2.5737e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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



## 5 Model quality

### 5.1 Standard geometry

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	0.38	0/1317	0.53	0/1770
1	B	0.40	0/1317	0.54	0/1770
1	C	0.37	0/1291	0.55	0/1736
1	D	0.39	0/1272	0.57	0/1710
1	E	0.35	0/1285	0.52	0/1727
1	F	0.36	0/1285	0.50	0/1727
All	All	0.37	0/7767	0.53	0/10440

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1295	0	1335	37	1
1	B	1295	0	1335	40	1
1	C	1269	0	1304	39	0
1	D	1250	0	1291	40	0
1	E	1263	0	1305	21	0
1	F	1263	0	1305	18	0
2	A	140	0	0	1	0
2	B	122	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	117	0	0	2	0
2	D	125	0	0	1	0
2	E	105	0	0	0	0
2	F	112	0	0	2	0
All	All	8356	0	7875	168	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 168 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:105:ILE:HG22	1:D:143:LEU:HD11	1.44	1.00
1:B:134:THR:HG22	1:B:136:GLU:H	1.29	0.94
1:A:134:THR:HG21	2:A:245:HOH:O	1.82	0.79
1:C:147:MET:HE3	1:D:146:PHE:HE1	1.44	0.79
1:A:85:ILE:HD11	1:A:122:VAL:HG21	1.67	0.76

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1:MET:O	1:B:1:MET:O[1_455]	1.93	0.27

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	167/176 (95%)	164 (98%)	2 (1%)	1 (1%)	33	24
1	B	167/176 (95%)	167 (100%)	0	0	100	100
1	C	164/176 (93%)	158 (96%)	4 (2%)	2 (1%)	19	9
1	D	161/176 (92%)	157 (98%)	4 (2%)	0	100	100
1	E	163/176 (93%)	160 (98%)	3 (2%)	0	100	100
1	F	163/176 (93%)	161 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	985/1056 (93%)	967 (98%)	15 (2%)	3 (0%)	50 44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	165	ALA
1	A	168	GLN
1	C	158	PRO

### 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	139/146 (95%)	131 (94%)	8 (6%)	28 21
1	B	139/146 (95%)	132 (95%)	7 (5%)	34 27
1	C	135/146 (92%)	129 (96%)	6 (4%)	39 32
1	D	134/146 (92%)	124 (92%)	10 (8%)	19 12
1	E	135/146 (92%)	125 (93%)	10 (7%)	20 12
1	F	135/146 (92%)	127 (94%)	8 (6%)	28 20
All	All	817/876 (93%)	768 (94%)	49 (6%)	27 20

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	104	LEU
1	D	141	GLN
1	F	132	LEU
1	D	132	LEU
1	D	157	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	168	GLN

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Mol	Chain	Res	Type
1	C	15	ASN
1	F	15	ASN
1	B	141	GLN
1	E	15	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

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, 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	169/176 (96%)	-0.39	4 (2%) 56 56	10, 17, 38, 59	0
1	B	169/176 (96%)	-0.28	3 (1%) 65 66	9, 19, 40, 56	0
1	C	166/176 (94%)	-0.19	7 (4%) 35 34	10, 19, 51, 75	0
1	D	163/176 (92%)	-0.16	8 (4%) 28 28	9, 19, 46, 70	0
1	E	165/176 (93%)	-0.26	4 (2%) 56 56	13, 22, 45, 69	0
1	F	165/176 (93%)	-0.21	6 (3%) 41 40	11, 21, 44, 73	0
All	All	997/1056 (94%)	-0.25	32 (3%) 45 45	9, 19, 46, 75	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	165	ALA	8.2
1	F	164	MET	7.0
1	D	162	LYS	6.6
1	C	165	ALA	6.5
1	E	165	ALA	5.8

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.