



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 02:09 am BST

PDB ID : 3BIC
Title : Crystal structure of human methylmalonyl-CoA mutase
Authors : Ugochukwu, E.; Kochan, G.; Pantic, N.; Parizotto, E.; Pilka, E.S.; Pike, A.C.W.; Gileadi, O.; von Delft, F.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.M.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2007-11-30
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

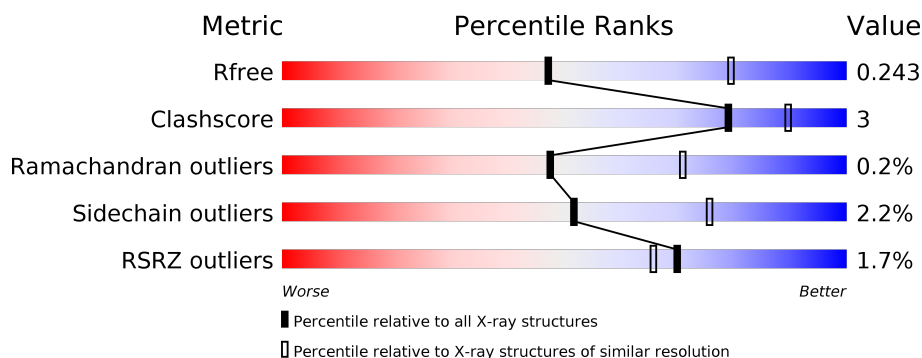
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	762	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	762	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10752 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 Methylmalonyl-CoA mutase, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	2	0
			5340	3396	908	1007	29			
1	B	715	Total	C	N	O	S	0	1	0
			5324	3376	909	1008	31			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	EXPRESSION TAG	UNP P22033
A	499	THR	ALA	VARIANT	UNP P22033
A	751	ALA	-	EXPRESSION TAG	UNP P22033
A	752	GLU	-	EXPRESSION TAG	UNP P22033
A	753	ASN	-	EXPRESSION TAG	UNP P22033
A	754	LEU	-	EXPRESSION TAG	UNP P22033
A	755	TYR	-	EXPRESSION TAG	UNP P22033
A	756	PHE	-	EXPRESSION TAG	UNP P22033
A	757	GLN	-	EXPRESSION TAG	UNP P22033
A	758	SER	-	EXPRESSION TAG	UNP P22033
A	759	HIS	-	EXPRESSION TAG	UNP P22033
A	760	HIS	-	EXPRESSION TAG	UNP P22033
A	761	HIS	-	EXPRESSION TAG	UNP P22033
A	762	HIS	-	EXPRESSION TAG	UNP P22033
A	763	HIS	-	EXPRESSION TAG	UNP P22033
A	764	HIS	-	EXPRESSION TAG	UNP P22033
A	765	ASP	-	EXPRESSION TAG	UNP P22033
A	766	TYR	-	EXPRESSION TAG	UNP P22033
A	767	LYS	-	EXPRESSION TAG	UNP P22033
A	768	ASP	-	EXPRESSION TAG	UNP P22033
A	769	ASP	-	EXPRESSION TAG	UNP P22033
A	770	ASP	-	EXPRESSION TAG	UNP P22033
A	771	ASP	-	EXPRESSION TAG	UNP P22033
A	772	LYS	-	EXPRESSION TAG	UNP P22033
B	11	MET	-	EXPRESSION TAG	UNP P22033

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	499	THR	ALA	VARIANT	UNP P22033
B	751	ALA	-	EXPRESSION TAG	UNP P22033
B	752	GLU	-	EXPRESSION TAG	UNP P22033
B	753	ASN	-	EXPRESSION TAG	UNP P22033
B	754	LEU	-	EXPRESSION TAG	UNP P22033
B	755	TYR	-	EXPRESSION TAG	UNP P22033
B	756	PHE	-	EXPRESSION TAG	UNP P22033
B	757	GLN	-	EXPRESSION TAG	UNP P22033
B	758	SER	-	EXPRESSION TAG	UNP P22033
B	759	HIS	-	EXPRESSION TAG	UNP P22033
B	760	HIS	-	EXPRESSION TAG	UNP P22033
B	761	HIS	-	EXPRESSION TAG	UNP P22033
B	762	HIS	-	EXPRESSION TAG	UNP P22033
B	763	HIS	-	EXPRESSION TAG	UNP P22033
B	764	HIS	-	EXPRESSION TAG	UNP P22033
B	765	ASP	-	EXPRESSION TAG	UNP P22033
B	766	TYR	-	EXPRESSION TAG	UNP P22033
B	767	LYS	-	EXPRESSION TAG	UNP P22033
B	768	ASP	-	EXPRESSION TAG	UNP P22033
B	769	ASP	-	EXPRESSION TAG	UNP P22033
B	770	ASP	-	EXPRESSION TAG	UNP P22033
B	771	ASP	-	EXPRESSION TAG	UNP P22033
B	772	LYS	-	EXPRESSION TAG	UNP P22033

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Cl 2 2	0	0
2	A	2	Total Cl 2 2	0	0

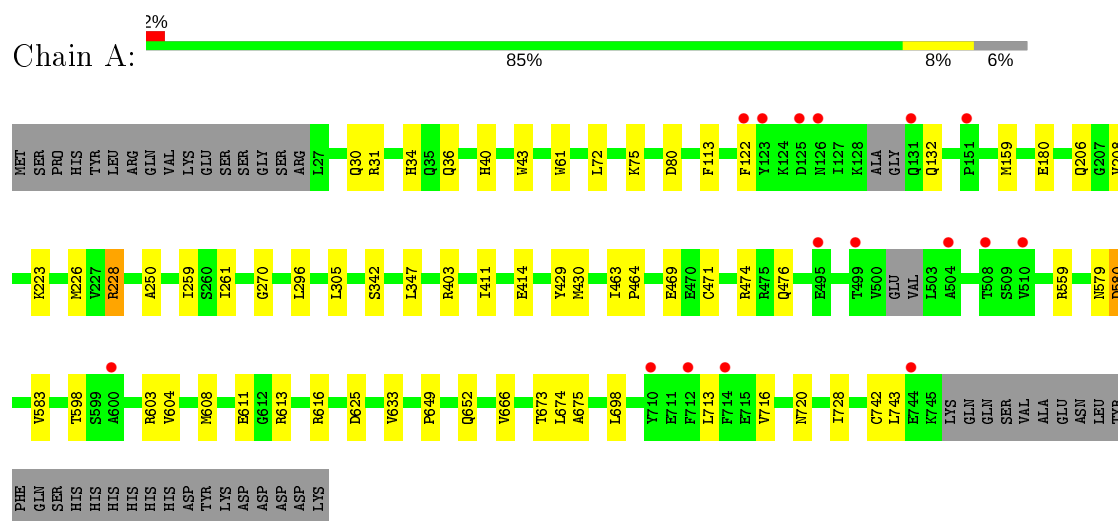
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	33	Total O 33 33	0	0
3	B	51	Total O 51 51	0	0

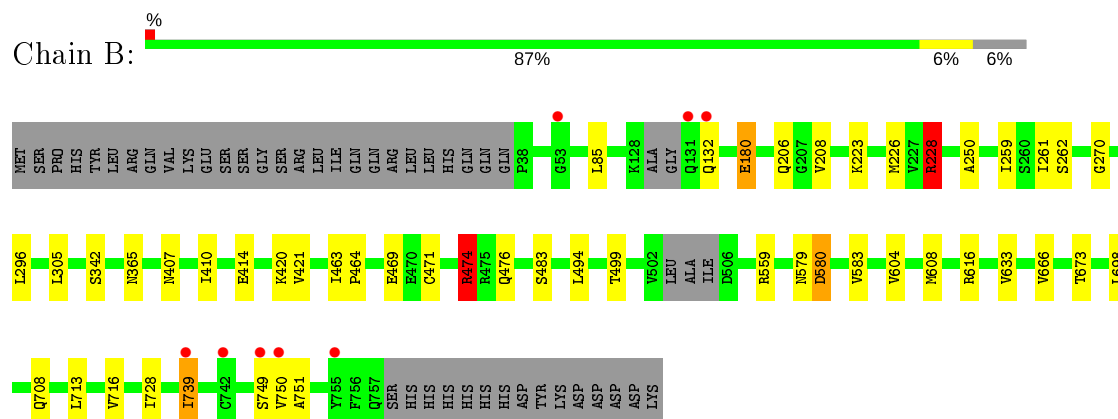
3 Residue-property plots [i](#)

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: Methylmalonyl-CoA mutase, mitochondrial precursor



- Molecule 1: Methylmalonyl-CoA mutase, mitochondrial precursor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.75Å 95.15Å 119.16Å 90.00° 108.31° 90.00°	Depositor
Resolution (Å)	37.42 – 2.60 37.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.42-2.60) 99.6 (37.43-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.217 , 0.243 0.221 , 0.243	Depositor DCC
R_{free} test set	1152 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10752	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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: CL

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	0/5451	0.68	7/7407 (0.1%)
1	B	0.42	0/5431	0.70	7/7382 (0.1%)
All	All	0.42	0/10882	0.69	14/14789 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	474	ARG	NE-CZ-NH2	-19.12	110.74	120.30
1	B	228	ARG	NE-CZ-NH1	-19.00	110.80	120.30
1	A	228	ARG	NE-CZ-NH2	-18.03	111.28	120.30
1	B	228	ARG	NE-CZ-NH2	15.60	128.10	120.30
1	A	228	ARG	NE-CZ-NH1	15.60	128.10	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	228	ARG	Sidechain
1	B	474	ARG	Sidechain

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	5340	0	5103	32	0
1	B	5324	0	5077	31	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	33	0	0	0	0
3	B	51	0	0	0	0
All	All	10752	0	10180	58	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 3.

The worst 5 of 58 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:579:ASN:HA	1:A:580:ASP:CB	2.01	0.91
1:B:579:ASN:HA	1:B:580:ASP:HB2	1.63	0.80
1:A:604:VAL:HG12	1:A:608:MET:CE	2.14	0.78
1:B:579:ASN:HA	1:B:580:ASP:CB	2.14	0.78
1:B:604:VAL:HG12	1:B:608:MET:CE	2.26	0.64

There are no symmetry-related clashes.

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	711/762 (93%)	691 (97%)	19 (3%)	1 (0%)	51	75
1	B	710/762 (93%)	687 (97%)	21 (3%)	2 (0%)	41	64
All	All	1421/1524 (93%)	1378 (97%)	40 (3%)	3 (0%)	47	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	580	ASP
1	B	580	ASP
1	B	750	VAL

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	520/636 (82%)	507 (98%)	13 (2%)	47	73
1	B	522/636 (82%)	512 (98%)	10 (2%)	57	79
All	All	1042/1272 (82%)	1019 (98%)	23 (2%)	52	76

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	613	ARG
1	A	720	ASN
1	B	673	THR
1	A	673	THR
1	B	132	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	ASN
1	B	407	ASN
1	B	132	GLN
1	A	132	GLN
1	A	605	HIS

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](#)

Of 4 ligands modelled in this entry, 4 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, 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	715/762 (93%)	-0.07	16 (2%) 62 56	30, 40, 56, 68	0
1	B	715/762 (93%)	-0.13	8 (1%) 80 78	29, 40, 55, 65	0
All	All	1430/1524 (93%)	-0.10	24 (1%) 70 66	29, 40, 55, 68	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	ALA	6.0
1	A	126	ASN	4.2
1	A	131	GLN	3.7
1	A	714	PHE	3.2
1	B	131	GLN	3.2

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. 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	B-factors(\AA^2)	Q<0.9
2	CL	A	803	1/1	0.80	0.13	78,78,78,78	0
2	CL	B	804	1/1	0.87	0.10	61,61,61,61	0
2	CL	A	801	1/1	0.98	0.21	45,45,45,45	0
2	CL	B	802	1/1	0.99	0.25	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.