

Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 05:57 PM EDT

PDB ID : 3VL3

Title : 3-isopropylmalate dehydrogenase from Shewanella oneidensis MR-1 at 340

MPa

Authors: Nagae, T.; Watanabe, N.

Deposited on : 2011-11-29

Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

Mol Probity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

 $\begin{tabular}{lll} CCP4 & : & 7.0.044 & (Gargrove) \end{tabular}$

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

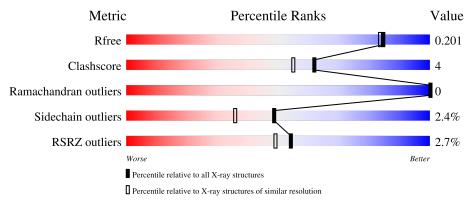
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.80 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 >=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 <=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	• •						
			3%							
1	A	375	80%	16%						



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3096 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 3-isopropylmalate dehydrogenase.

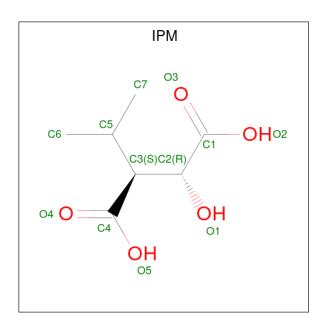
\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	A	364	Total 2807	C 1762	N 490	O 537	S 18	0	9	0	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q8E9N3
A	-9	ARG	-	expression tag	UNP Q8E9N3
A	-8	GLY	-	expression tag	UNP Q8E9N3
A	-7	SER	-	expression tag	UNP Q8E9N3
A	-6	HIS	-	expression tag	UNP Q8E9N3
A	-5	HIS	-	expression tag	UNP Q8E9N3
A	-4	HIS	-	expression tag	UNP Q8E9N3
A	-3	HIS	-	expression tag	UNP Q8E9N3
A	-2	HIS	-	expression tag	UNP Q8E9N3
A	-1	HIS	-	expression tag	UNP Q8E9N3
A	0	GLY	-	expression tag	UNP Q8E9N3
A	1	SER	-	expression tag	UNP Q8E9N3

• Molecule 2 is 3-ISOPROPYLMALIC ACID (three-letter code: IPM) (formula: $C_7H_{12}O_5$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 12	C 7	O 5	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0

• Molecule 5 is water.

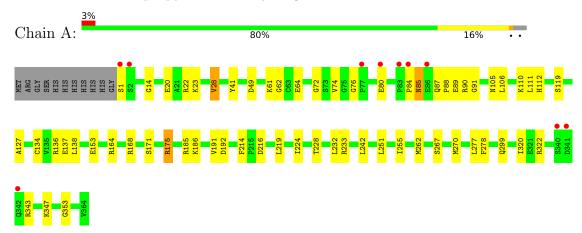
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	275	Total O 275 275	0	0



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: 3-isopropylmalate dehydrogenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	103.82Å 57.88Å 75.67Å	Donositon
a, b, c, α , β , γ	90.00° 119.02° 90.00°	Depositor
Resolution (Å)	33.09 - 1.80	Depositor
Resolution (A)	33.09 - 1.80	EDS
% Data completeness	91.3 (33.09-1.80)	Depositor
(in resolution range)	91.3 (33.09-1.80)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	5.76 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
D D	0.157 , 0.202	Depositor
R, R_{free}	0.156 , 0.201	DCC
R_{free} test set	1680 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 39.6	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
	0.015 for 1/2 *h-3/2 *k,-1/2 *h-1/2 *k,-1/2 *h	
Estimated twinning fraction	+1/2*k-l 0.022 for $1/2$ *h $+3/2$ *k, $1/2$ *h- $1/2$ *k, $-1/2$ *h-	Xtriage
E E completion	1/2*k-l	EDC
F_o, F_c correlation	0.97	EDS
Total number of atoms	3096	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.85% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: IPM, CA, 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	Boı	nd lengths	Во	ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	1.38	8/2881 (0.3%)	1.23	18/3885 (0.5%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	A	137	GLU	CB-CG	7.87	1.67	1.52
1	A	214	PHE	CE1-CZ	6.46	1.49	1.37
1	A	191	VAL	CB-CG2	5.58	1.64	1.52
1	A	278	PHE	CE1-CZ	5.53	1.47	1.37
1	A	185	ARG	CZ-NH1	5.41	1.40	1.33
1	A	127	ALA	CA-CB	5.34	1.63	1.52
1	A	14	GLY	N-CA	5.29	1.53	1.46
1	A	23	LYS	CD-CE	5.13	1.64	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}(^{o})$
1	A	185	ARG	NE-CZ-NH2	-10.65	114.97	120.30
1	A	322	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	49	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	219	LEU	CB-CG-CD1	-6.47	100.00	111.00
1	A	185	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	136	ARG	NE-CZ-NH1	-6.21	117.20	120.30
1	A	175[A]	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	A	175[B]	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	A	164	ARG	CG-CD-NE	6.06	124.52	111.80
1	A	168	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	262	MET	CA-CB-CG	-5.88	103.30	113.30
1	A	22	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	A	192	ASP	CB-CG-OD1	5.67	123.41	118.30

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Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	242	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	A	251	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	A	267	SER	N-CA-CB	-5.20	102.70	110.50
1	A	347	LYS	CD-CE-NZ	-5.06	100.06	111.70
1	A	232	LEU	CB-CG-CD2	-5.03	102.45	111.00

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	2807	0	2823	25	0
2	A	12	0	9	1	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	275	0	0	1	0
All	All	3096	0	2832	25	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 4.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:84:PRO:HA	1:A:87:GLN:OE1	1.71	0.89
1:A:85:ASN:HA	1:A:90:ARG:HD3	1.67	0.74
1:A:87:GLN:HG3	1:A:88:PRO:HD2	1.80	0.62
1:A:171:SER:O	1:A:175[B]:ARG:HG3	2.00	0.62
1:A:224:ILE:O	1:A:228:THR:HG23	1.99	0.62
1:A:105:ASN:HB2	1:A:138:LEU:HD22	1.81	0.61
1:A:72:GLY:HA2	1:A:299:GLN:HE22	1.67	0.60
1:A:106:LEU:HD12	1:A:270[A]:MET:HE1	1.85	0.57
1:A:85:ASN:N	1:A:85:ASN:OD1	2.41	0.53
1:A:20:GLU:OE1	1:A:353:GLY:HA3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:HG3	1:A:91:GLY:N	2.25	0.52
1:A:186:LYS:HD3	1:A:216:ASP:O	2.10	0.52
1:A:134[B]:CYS:SG	1:A:255:ILE:HD12	2.51	0.50
1:A:111:LEU:HD21	1:A:119:SER:HB2	1.95	0.48
1:A:80:GLU:HA	1:A:87:GLN:NE2	2.30	0.47
1:A:87:GLN:CG	1:A:88:PRO:HD2	2.45	0.45
1:A:41:TYR:CZ	1:A:62:GLY:HA3	2.53	0.44
1:A:74:VAL:HG23	1:A:89[A]:GLU:HA	2.00	0.44
1:A:74:VAL:HG23	1:A:89[B]:GLU:HA	2.00	0.43
1:A:28:VAL:HG21	1:A:320:ILE:HG13	2.01	0.43
1:A:277:LEU:C	1:A:277:LEU:HD23	2.40	0.42
1:A:76:GLY:O	1:A:80:GLU:HG3	2.19	0.42
1:A:61:LYS:HE3	1:A:64:GLU:OE1	2.20	0.41
1:A:112:HIS:HB3	5:A:680:HOH:O	2.21	0.41
1:A:89[B]:GLU:HG2	2:A:401:IPM:H62	2.01	0.41

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	371/375 (99%)	359 (97%)	12 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	Analysed Rotameric Outliers		Percentiles	
1	A	297/297 (100%)	290 (98%)	7 (2%)	49 36	

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	28	VAL
1	A	85	ASN
1	A	110	LYS
1	A	153	GLU
1	A	233	ARG
1	A	343	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	299	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The



Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

	Mol	l Type Chai		Res	Link	Bond lengths			Bond angles		
	IVIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
Ī	2	IPM	A	401	3	11,11,11	1.98	4 (36%)	10,15,15	1.44	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IPM	A	401	3	-	1/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(ext{\AA})$
2	A	401	IPM	C3-C5	-4.59	1.46	1.55
2	A	401	IPM	C3-C2	-2.48	1.51	1.54
2	A	401	IPM	C6-C5	2.26	1.60	1.52
2	A	401	IPM	C3-C4	2.02	1.56	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	401	IPM	O4-C4-C3	-2.90	115.05	122.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	IPM	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

\mathbf{Mol}	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	IPM	1	0



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^{th} 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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	364/375 (97%)	-0.37	10 (2%) 54 49	8, 15, 39, 56	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	6.0
1	A	84	PRO	4.0
1	A	340	SER	3.6
1	A	83	PRO	3.4
1	A	2	SER	3.3
1	A	341	ASP	3.1
1	A	86	GLU	2.9
1	A	77	PRO	2.5
1	A	80	GLU	2.3
1	A	342	GLN	2.1

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 monosaccharides 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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	IPM	A	401	12/12	0.98	0.11	8,11,17,17	0
4	CL	A	403	1/1	0.99	0.10	11,11,11,11	0
3	CA	A	402	1/1	1.00	0.07	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.

