

wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 09:06 am BST

PDB ID : 3WZY

Title: S266A mutant 3-isopropylmalate dehydrogenase from Shewanella oneidensis

MR-1 at 580MPa - complex with IPM and Mg

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Deposited on : 2014-10-08

Resolution : 1.55 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 (i) symbol.

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

MolProbity : 4.02b-467

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

Xtriage (Phenix) : 1.13 EDS : 2.11

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

Refmac: 5.8.0158

 $\begin{array}{cccc} & CCP4 & : & 7.0.044 \; (Gargrove) \\ Ideal \; geometry \; (proteins) & : & Engh \; \& \; Huber \; (2001) \end{array}$

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

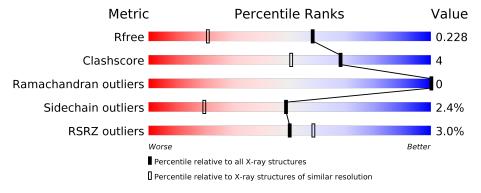
Validation Pipeline (wwPDB-VP) : 2.11

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 1.55 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 <=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	86%	11%	•



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3107 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.

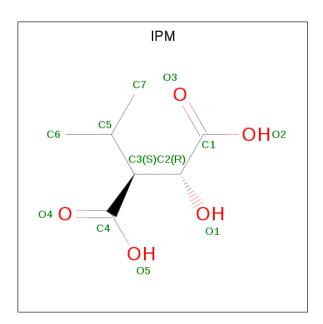
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	364	Total 2766	C 1735	N 488	O 527	S 16	0	1	0

There are 13 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
A	266	ALA	SER	ENGINEERED MUTATION	UNP Q8E9N3

• Molecule 2 is 3-ISOPROPYLMALIC ACID (three-letter code: IPM) (formula: C₇H₁₂O₅).





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

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg	0	0

• Molecule 4 is water.

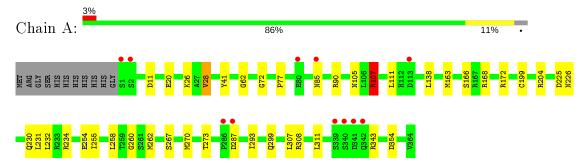
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	328	Total O 328 328	0	0



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: 3-isopropylmalate dehydrogenase





4 Data and refinement statistics (i)

Property	Value	Source		
Space group	C 1 2 1	Depositor		
Cell constants	102.31Å 57.42Å 75.36Å	D : 4		
a, b, c, α , β , γ	90.00° 118.81° 90.00°	Depositor		
Resolution (Å)	36.18 - 1.55	Depositor		
Resolution (A)	36.18 - 1.55	EDS		
% Data completeness	90.5 (36.18-1.55)	Depositor		
(in resolution range)	90.5 (36.18-1.55)	EDS		
R_{merge}	0.06	Depositor		
R_{sym}	(Not available)	Depositor		
$< I/\sigma(I) > 1$	2.44 (at 1.55Å)	Xtriage		
Refinement program	REFMAC 5.8.0073	Depositor		
D D	0.185 , 0.222	Depositor		
R, R_{free}	0.197 , 0.228	DCC		
R_{free} test set	2587 reflections (5.12%)	wwPDB-VP		
Wilson B-factor (\mathring{A}^2)	16.1	Xtriage		
Anisotropy	0.021	Xtriage		
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37, 34.2	EDS		
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage		
	0.009 for 1/2 +h-3/2 +k,-1/2 +h-1/2 +k,-1/2 +h			
Estimated twinning fraction	+1/2*k-1	Xtriage		
	0.026 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-	11011080		
E E completion	1/2*k-l	EDC		
F_o, F_c correlation	0.96	EDS		
Total number of atoms	3107	wwPDB-VP		
Average B, all atoms (\mathring{A}^2)	21.0	wwPDB-VP		

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.33% 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.



 $^{^{1}}$ Intensities 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: MG, IPM

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).

Mal	Chain	Bo	nd lengths	Bond angles		
MIOI	$ig \operatorname{\mathbf{Mol}} ig \operatorname{\mathbf{Chain}} ig _{\operatorname{R}}$		# Z > 5	RMSZ # Z > 5		
1	A	1.11	3/2816 (0.1%)	1.19	$14/3799 \ (0.4\%)$	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
1	A	267	SER	CB-OG	-6.61	1.33	1.42
1	A	254	GLU	CD-OE1	-5.36	1.19	1.25
1	A	166	SER	CA-CB	-5.06	1.45	1.52

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

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathbf{Ideal}(^o)$
1	A	11	ASP	CB-CG-OD1	-8.52	110.63	118.30
1	A	11	ASP	CB-CG-OD2	7.90	125.41	118.30
1	A	172	ARG	NE-CZ-NH1	-6.97	116.82	120.30
1	A	225	ASP	CB-CG-OD1	6.96	124.57	118.30
1	A	354	ASP	CB-CG-OD2	-6.96	112.04	118.30

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	Α	2766	0	2772	21	0
2	A	12	0	9	0	0
3	A	1	0	0	0	0
4	A	328	0	0	6	0
All	All	3107	0	2781	21	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.

The worst 5 of 21 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{l} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:260:GLY:HA2	4:A:819:HOH:O	1.48	1.13
1:A:77:PRO:HG2	4:A:815:HOH:O	1.82	0.78
1:A:72:GLY:HA2	1:A:299:GLN:HE22	1.52	0.74
1:A:260:GLY:CA	4:A:819:HOH:O	2.23	0.67
1:A:231:LEU:HD13	1:A:255:ILE:HG13	1.89	0.54

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	Perce	$_{ m ntiles}$
1	A	363/375~(97%)	355 (98%)	8 (2%)	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	288/296 (97%)	280 (97%)	8 (3%)	43 14

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107[A]	ARG
1	A	293	ILE
1	A	111	LEU
1	A	90	ARG
1	A	107[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	105	ASN
1	A	226	ASN
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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is 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		Type	Chain	Res	Link	B	ond leng	gths	В	ond ang	gles
	MIOI	туре	Chain	res	LIIIK	Counts	RMSZ	# Z > 2	Counts RMSZ $\# Z > 2$		
	2	IPM	A	401	3	5,11,11	1.64	1 (20%)	5,15,15	1.11	0

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	-	0/8/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed(\AA)}$	$\operatorname{Ideal}(\operatorname{\AA})$
2	Α	401	IPM	C3-C2	-3.29	1.50	1.54

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, 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	<RSRZ $>$	$>$ #RSRZ $>$ 2 OWAB($ m \AA^2$)		Q < 0.9
1	A	364/375 (97%)	-0.01	11 (3%) 50 58	10, 17, 39, 61	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	7.1
1	A	341	ASP	5.2
1	A	2	SER	4.1
1	A	340	SER	3.4
1	A	286	PRO	2.8

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)

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	${f B-factors}({f A}^2)$	Q<0.9
2	IPM	A	401	12/12	0.97	0.09	10,14,16,17	0
3	MG	A	402	1/1	0.99	0.08	10,10,10,10	0



6.5 Other polymers (i)

There are no such residues in this entry.

