



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 10:11 pm BST

PDB ID : 2J5R
Title : 2.25 Å resolution structure of the wild type malate dehydrogenase from *Haloarcula marismortui* after second radiation burn (radiation damage series)
Authors : Fioravanti, E.; Vellieux, F.M.D.; Amara, P.; Madern, D.; Weik, M.
Deposited on : 2006-09-19
Resolution : 2.25 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

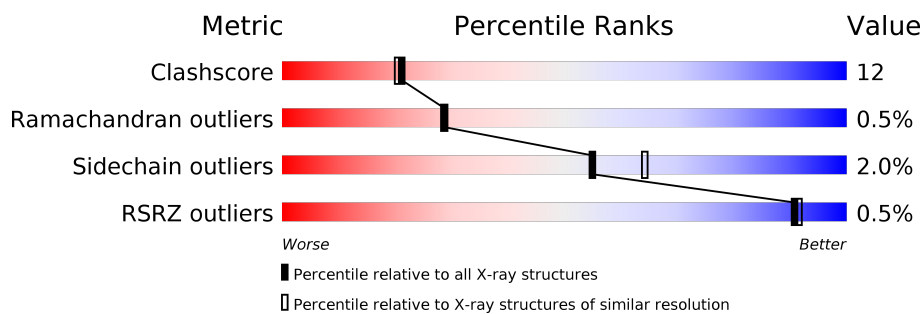
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	304	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div> </div>
1	B	304	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>
1	C	304	<div> <div></div> <div> <div>78%</div> <div>21%</div> <div>.</div> </div> </div>
1	D	304	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	1333	-	-	X	-
2	CL	B	1332	-	-	X	-
2	CL	C	1332	-	-	X	-
2	CL	D	1331	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10082 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 MALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2278	1406	391	477	4			
1	B	298	Total	C	N	O	S	0	0	0
			2240	1383	383	470	4			
1	C	303	Total	C	N	O	S	0	0	0
			2285	1409	393	479	4			
1	D	298	Total	C	N	O	S	0	0	0
			2248	1387	383	474	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cl	0	0
			2	2		
2	A	3	Total	Cl	0	0
			3	3		
2	D	1	Total	Cl	0	0
			1	1		
2	C	2	Total	Cl	0	0
			2	2		

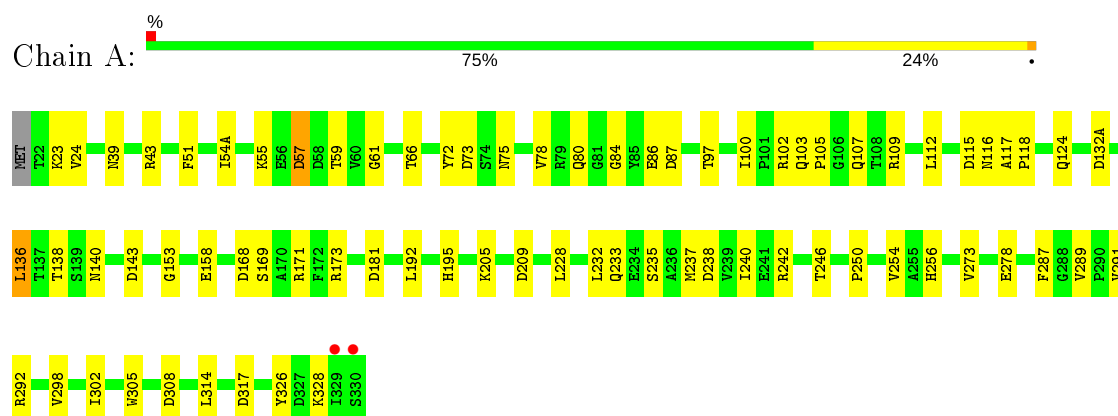
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	265	Total	O	0	0
			265	265		
3	B	230	Total	O	0	0
			230	230		
3	C	259	Total	O	0	0
			259	259		
3	D	269	Total	O	0	0
			269	269		

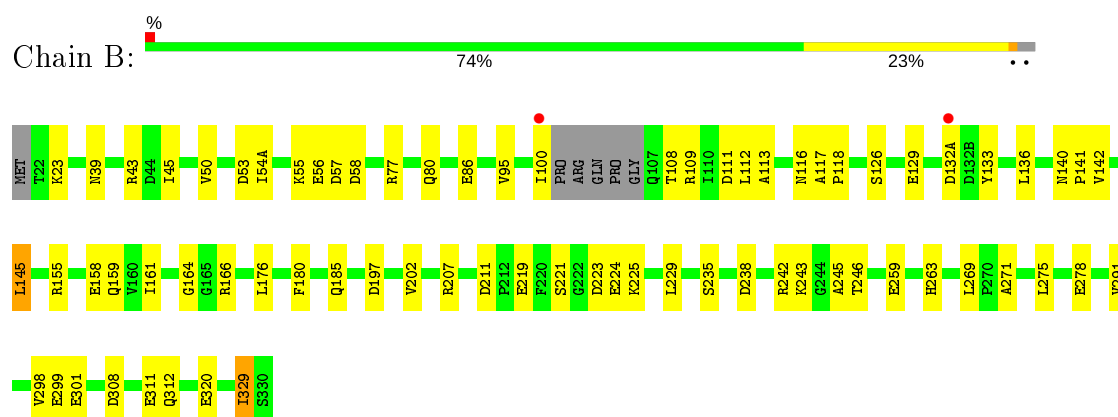
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

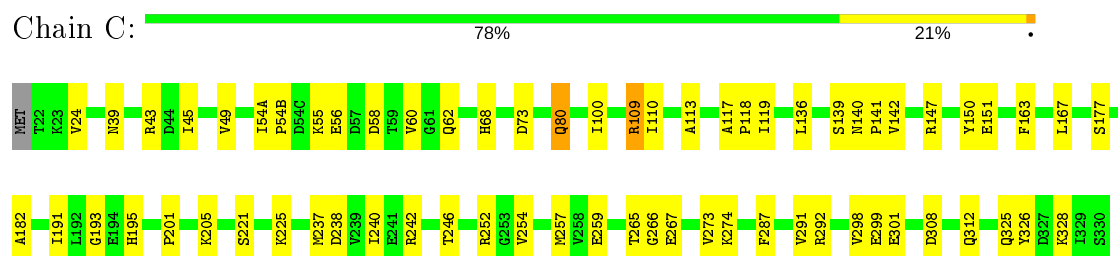
• Molecule 1: MALATE DEHYDROGENASE



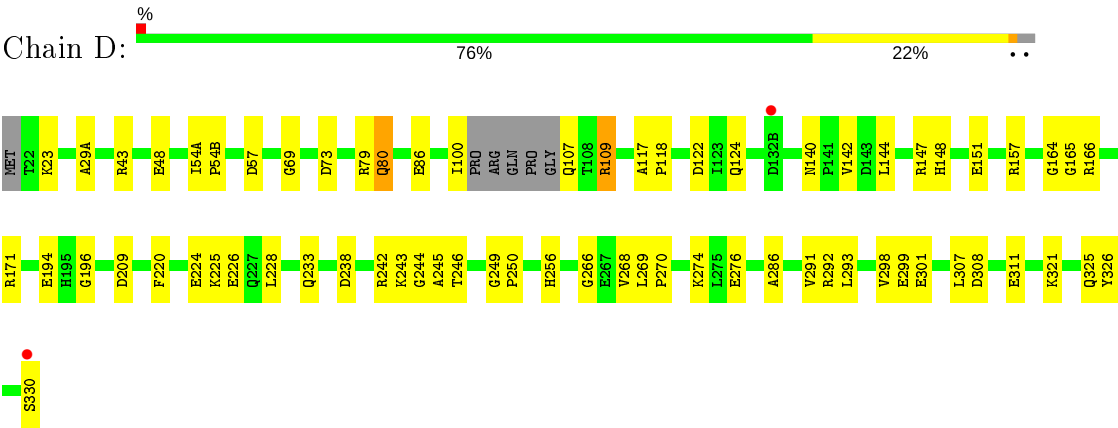
• Molecule 1: MALATE DEHYDROGENASE



• Molecule 1: MALATE DEHYDROGENASE



• Molecule 1: MALATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.38Å 114.57Å 124.53Å 90.00° 93.34° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 19.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.25) 81.1 (19.99-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.271 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10082	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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

5.1 Standard geometry

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	0.52	0/2313	0.68	0/3139
1	B	0.49	0/2274	0.69	0/3087
1	C	0.52	0/2322	0.71	0/3154
1	D	0.50	0/2282	0.71	0/3097
All	All	0.51	0/9191	0.70	0/12477

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	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	TYR	Sidechain
1	C	326	TYR	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	2278	0	2144	57	0
1	B	2240	0	2106	53	0
1	C	2285	0	2153	52	0
1	D	2248	0	2114	59	0
2	A	3	0	0	2	0
2	B	2	0	0	3	0
2	C	2	0	0	2	0
2	D	1	0	0	2	0
3	A	265	0	0	9	0
3	B	230	0	0	12	0
3	C	259	0	0	6	0
3	D	269	0	0	10	0
All	All	10082	0	8517	213	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 12.

The worst 5 of 213 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:103:GLN:O	1:A:105:PRO:N	1.86	1.08
1:A:140:ASN:HB2	3:A:2118:HOH:O	1.62	0.97
1:C:238:ASP:HA	1:C:242:ARG:HD2	1.56	0.88
1:A:181:ASP:HB2	3:A:2146:HOH:O	1.73	0.87
1:D:86:GLU:CD	1:D:86:GLU:H	1.81	0.82

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	299/304 (98%)	286 (96%)	12 (4%)	1 (0%)	41	46
1	B	294/304 (97%)	279 (95%)	12 (4%)	3 (1%)	15	13
1	C	301/304 (99%)	286 (95%)	15 (5%)	0	100	100
1	D	294/304 (97%)	280 (95%)	12 (4%)	2 (1%)	22	21
All	All	1188/1216 (98%)	1131 (95%)	51 (4%)	6 (0%)	29	29

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132(A)	ASP
1	B	164	GLY
1	A	132(A)	ASP
1	D	29(A)	ALA
1	D	164	GLY

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	237/245 (97%)	233 (98%)	4 (2%)	60	71
1	B	233/245 (95%)	226 (97%)	7 (3%)	41	50
1	C	239/245 (98%)	236 (99%)	3 (1%)	69	79
1	D	235/245 (96%)	230 (98%)	5 (2%)	53	62
All	All	944/980 (96%)	925 (98%)	19 (2%)	55	64

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	145	LEU
1	B	223	ASP
1	D	80	GLN

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Mol	Chain	Res	Type
1	B	80	GLN
1	D	109	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	199	GLN
1	C	80	GLN
1	D	80	GLN
1	B	159	GLN
1	C	325	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 8 ligands modelled in this entry, 8 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	303/304 (99%)	-0.10	2 (0%) 87 88	11, 22, 35, 59	0
1	B	298/304 (98%)	-0.10	2 (0%) 87 88	12, 23, 41, 55	0
1	C	303/304 (99%)	-0.12	0 100 100	9, 21, 33, 47	0
1	D	298/304 (98%)	-0.08	2 (0%) 87 88	11, 23, 37, 57	0
All	All	1202/1216 (98%)	-0.10	6 (0%) 91 91	9, 22, 37, 59	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	SER	3.2
1	D	132(B)	ASP	2.7
1	B	100	ILE	2.4
1	B	132(A)	ASP	2.2
1	A	329	ILE	2.2

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	D	1331	1/1	0.96	0.24	52,52,52,52	0
2	CL	B	1332	1/1	0.96	0.72	78,78,78,78	0
2	CL	A	1331	1/1	0.98	0.09	17,17,17,17	0
2	CL	C	1332	1/1	0.98	0.13	36,36,36,36	0
2	CL	A	1333	1/1	0.98	0.18	43,43,43,43	0
2	CL	A	1332	1/1	0.99	0.06	26,26,26,26	0
2	CL	B	1331	1/1	0.99	0.09	22,22,22,22	0
2	CL	C	1331	1/1	0.99	0.10	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.