wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 11:25 PM EDT

PDB ID	:	2A9F
Title	:	Crystal structure of a putative malic enzyme ((S)-malate:NAD+ oxidoreductase (decarboxylating))
Authors	:	Seetharaman, J.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2005-07-11
Resolution	:	2.50 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 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:

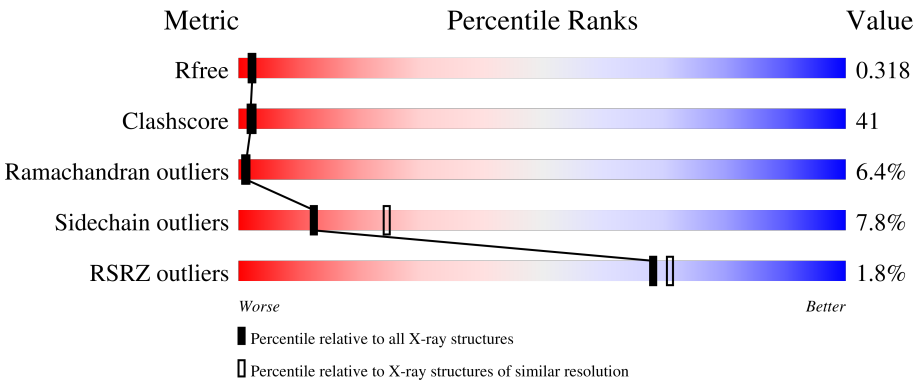
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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
1	A	398	2%, 42%, 47%, 7% • •
1	B	398	2%, 44%, 41%, 9% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5614 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 putative malic enzyme ((S)-malate:NAD+ oxidoreductase (decarboxylating)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	2793	1783	464	539	7	0	0	0
1	B	380	2770	1767	459	537	7	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q99ZS1
A	2	SER	-	cloning artifact	UNP Q99ZS1
A	3	LEU	-	cloning artifact	UNP Q99ZS1
A	391	GLU	-	cloning artifact	UNP Q99ZS1
A	392	GLY	-	cloning artifact	UNP Q99ZS1
A	393	HIS	-	expression tag	UNP Q99ZS1
A	394	HIS	-	expression tag	UNP Q99ZS1
A	395	HIS	-	expression tag	UNP Q99ZS1
A	396	HIS	-	expression tag	UNP Q99ZS1
A	397	HIS	-	expression tag	UNP Q99ZS1
A	398	HIS	-	expression tag	UNP Q99ZS1
B	1	MET	-	cloning artifact	UNP Q99ZS1
B	2	SER	-	cloning artifact	UNP Q99ZS1
B	3	LEU	-	cloning artifact	UNP Q99ZS1
B	391	GLU	-	cloning artifact	UNP Q99ZS1
B	392	GLY	-	cloning artifact	UNP Q99ZS1
B	393	HIS	-	expression tag	UNP Q99ZS1
B	394	HIS	-	expression tag	UNP Q99ZS1
B	395	HIS	-	expression tag	UNP Q99ZS1
B	396	HIS	-	expression tag	UNP Q99ZS1
B	397	HIS	-	expression tag	UNP Q99ZS1
B	398	HIS	-	expression tag	UNP Q99ZS1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
			Total	Mg		
2	B	1	1	1	0	0

- Molecule 3 is water.

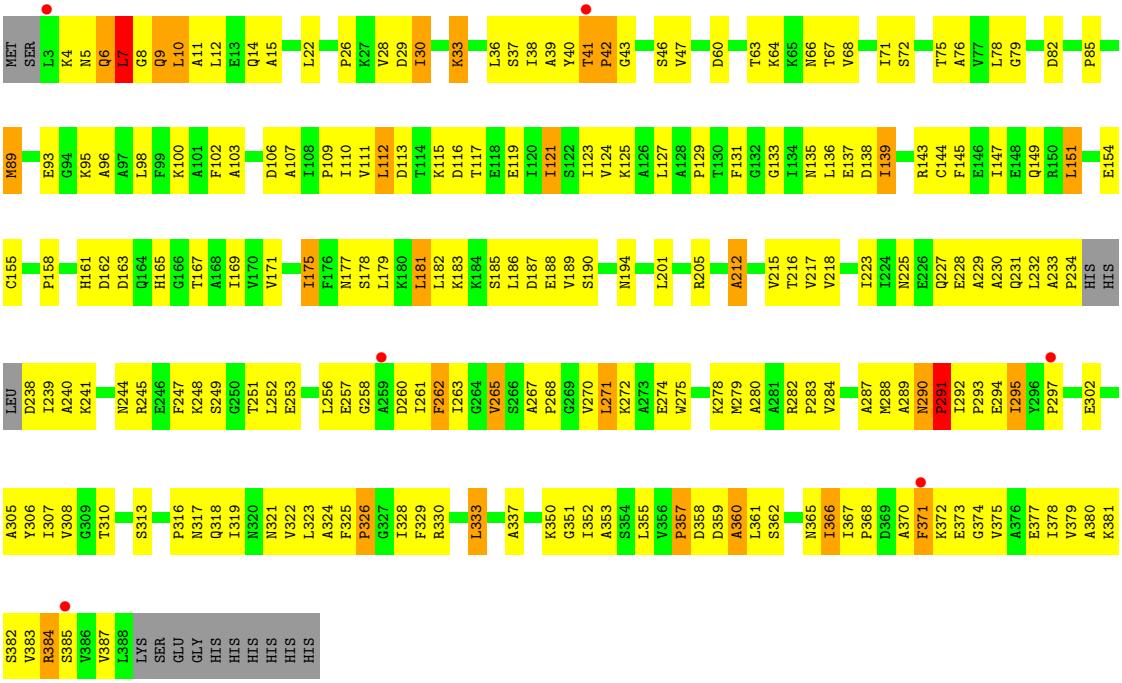
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	24	24	24	0	0
			Total	O		
3	B	25	25	25	0	0

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.

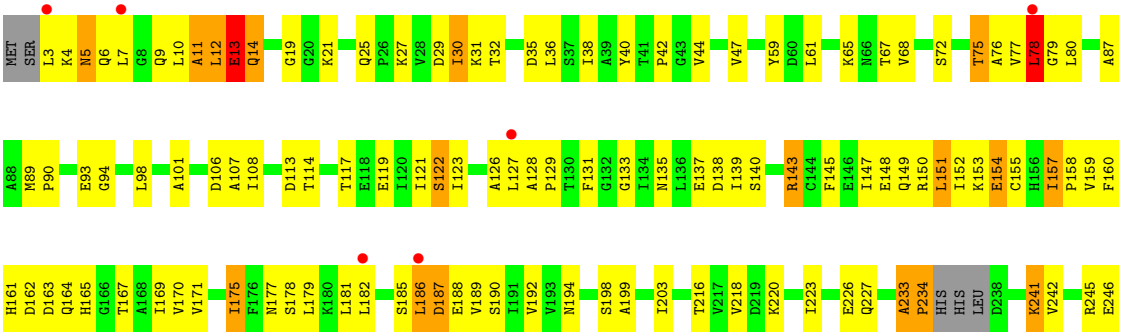
• Molecule 1: putative malic enzyme ((S)-malate:NAD+ oxidoreductase (decarboxylating))

Chain A:



• Molecule 1: putative malic enzyme ((S)-malate:NAD+ oxidoreductase (decarboxylating))

Chain B:



F247 K248 S249 G250 T251 L252 E253
L256 E257 G258 A259 D260 I261 F262 I263 G264 V265 S266 A267 P268 G269 V270 L271 K272 A273 E274 W275 I276
M279 A280
P283 V284 I285 F286 A287 M288 A289 N290 P291
E294 I295 Y296 P297 D298 E299 A300
A303
I307 V308 G309 T310 G311 R312 S313
D314 F315 P316 N317 Q318 I319 N320 N321 V322 L323 A324 F325 P326 G327 I328 F329
L333
R336 A337 K338 T339 I340 T341 V342 E343 M344 Q345 I346 A347
G351 I352 A353 S354 L355 V356 P357 D358 D359 A360 L361 S362 T363 T364 N365 I366 I367 P368
G374
I378 V379 A380 K381
R384 S385
VAL VAL LEU LYS SER GLU GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.26Å 79.25Å 145.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 2.50 49.79 – 2.48	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.79-2.50) 92.9 (49.79-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.260 , 0.304 0.271 , 0.318	Depositor DCC
R_{free} test set	1016 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5614	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

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

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	0.43	0/2832	0.75	1/3846 (0.0%)
1	B	0.44	0/2809	0.77	6/3817 (0.2%)
All	All	0.43	0/5641	0.76	7/7663 (0.1%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	234	PRO	N-CA-CB	5.82	110.28	103.30
1	A	234	PRO	N-CA-CB	5.66	110.09	103.30
1	B	78	LEU	CA-C-N	-5.63	104.94	116.20
1	B	14	GLN	N-CA-C	-5.58	95.94	111.00
1	B	333	LEU	CA-CB-CG	5.52	127.99	115.30

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	A	2793	0	2856	238	0
1	B	2770	0	2826	263	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	0	0	2	0
3	B	25	0	0	1	0
All	All	5614	0	5682	462	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 41.

The worst 5 of 462 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:B:341:THR:H	1:B:344:MET:HE3	1.02	1.16
1:A:189:VAL:HA	1:A:261:ILE:HD12	1.28	1.13
1:A:290:ASN:HB2	1:A:291:PRO:HD2	1.31	1.12
1:B:128:ALA:HB1	1:B:157:ILE:HD12	1.41	1.02
1:A:238:ASP:HA	1:A:241:LYS:HD2	1.47	0.96

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	379/398 (95%)	309 (82%)	46 (12%)	24 (6%)	1 1
1	B	376/398 (94%)	315 (84%)	37 (10%)	24 (6%)	1 1
All	All	755/796 (95%)	624 (83%)	83 (11%)	48 (6%)	1 1

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	7	LEU

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Mol	Chain	Res	Type
1	A	41	THR
1	A	232	LEU
1	A	233	ALA

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	Rotameric	Outliers	Percentiles	
1	A	289/314 (92%)	268 (93%)	21 (7%)	14	27
1	B	287/314 (91%)	263 (92%)	24 (8%)	11	21
All	All	576/628 (92%)	531 (92%)	45 (8%)	12	24

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	155	CYS
1	B	256	LEU
1	B	157	ILE
1	B	241	LYS
1	B	274	GLU

Sometimes 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	14	GLN
1	B	25	GLN
1	B	321	ASN
1	B	177	ASN
1	B	194	ASN

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 2 ligands modelled in this entry, 2 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	383/398 (96%)	0.03	6 (1%)	72	74	36, 56, 74, 94	0
1	B	380/398 (95%)	0.03	8 (2%)	63	66	36, 56, 75, 88	0
All	All	763/796 (95%)	0.03	14 (1%)	68	71	36, 56, 75, 94	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	LEU	4.7
1	B	368	PRO	4.0
1	B	3	LEU	3.9
1	A	259	ALA	3.6
1	B	186	LEU	3.5

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, 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(Å^2)	Q<0.9
2	MG	A	801	1/1	0.98	0.19	27,27,27,27	0
2	MG	B	800	1/1	0.98	0.14	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.