



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:50 pm GMT

PDB ID : 1GV1
Title : STRUCTURAL BASIS FOR THERMOPHILIC PROTEIN STABILITY:
STRUCTURES OF THERMOPHILIC AND MESOPHILIC MALATE DE-
HYDROGENASES
Authors : Dalhus, B.; Sarinen, M.; Sauer, U.H.; Eklund, P.; Johansson, K.; Karlsson, A.;
Ramaswamy, S.; Bjork, A.; Synstad, B.; Naterstad, K.; Sirevag, R.; Eklund,
H.
Deposited on : 2002-02-04
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

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

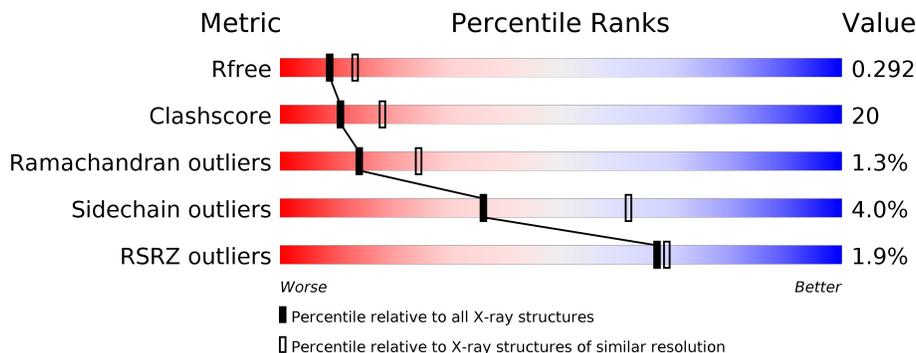
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	310	
1	B	310	
1	C	310	
1	D	310	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9395 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
			Total	C	N	O	S			
1	A	305	2293	1451	391	436	15	0	0	0
1	B	290	2172	1378	367	415	12	0	0	0
1	C	305	2293	1451	391	436	15	0	0	0
1	D	292	2187	1386	370	418	13	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	ALA	SER	CONFLICT	UNP P80039
A	229	ALA	GLY	CONFLICT	UNP P80039
B	227	ALA	SER	CONFLICT	UNP P80039
B	229	ALA	GLY	CONFLICT	UNP P80039
C	227	ALA	SER	CONFLICT	UNP P80039
C	229	ALA	GLY	CONFLICT	UNP P80039
D	227	ALA	SER	CONFLICT	UNP P80039
D	229	ALA	GLY	CONFLICT	UNP P80039

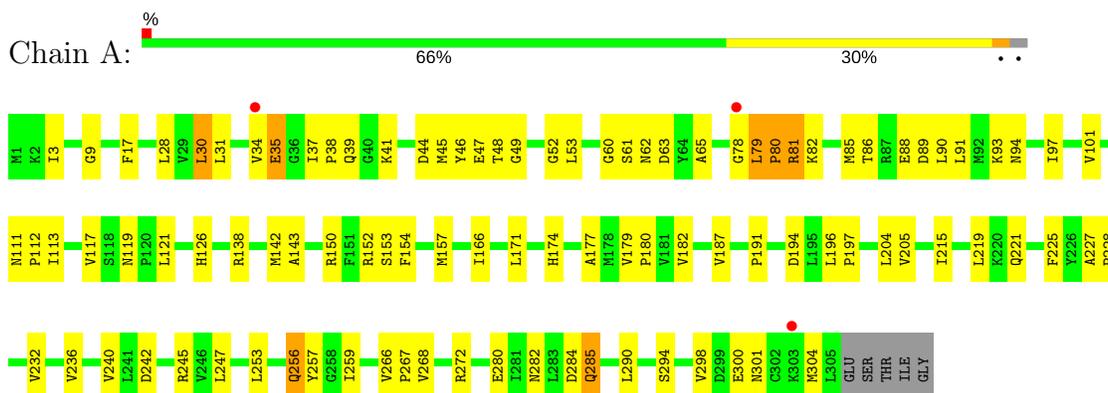
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	135	Total 135	O 135	0	0
2	B	78	Total 78	O 78	0	0
2	C	115	Total 115	O 115	0	0
2	D	122	Total 122	O 122	0	0

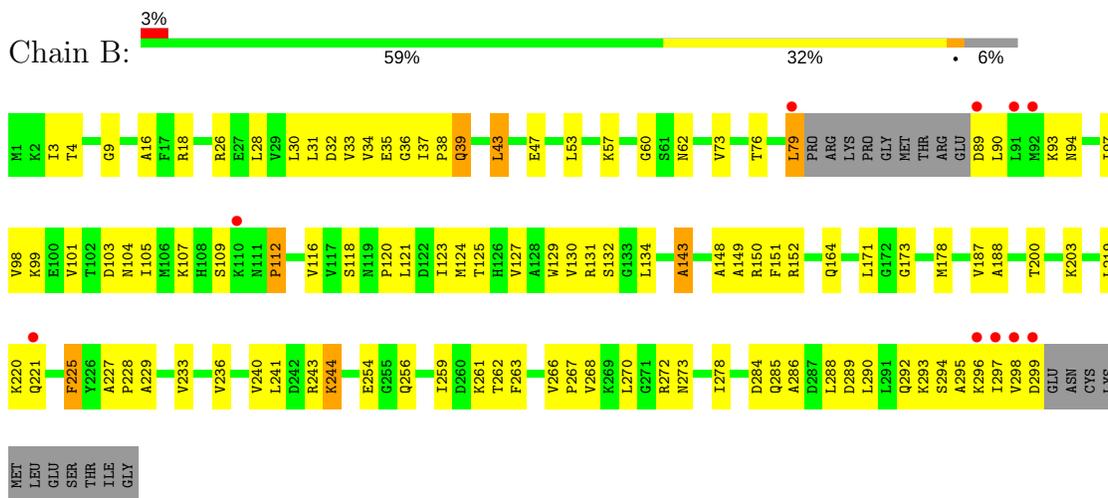
3 Residue-property plots [i](#)

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: MALATE DEHYDROGENASE



• Molecule 1: MALATE DEHYDROGENASE



• Molecule 1: MALATE DEHYDROGENASE





● Molecule 1: MALATE DEHYDROGENASE



ILE
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.42Å 85.82Å 117.50Å 90.00° 104.61° 90.00°	Depositor
Resolution (Å)	19.92 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.0 (19.92-2.50) 88.1 (19.97-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.50Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.305 0.208 , 0.292	Depositor DCC
R_{free} test set	3814 reflections (10.09%)	DCC
Wilson B-factor (Å ²)	24.9	Xtrriage
Anisotropy	0.794	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9395	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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](#)

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	0.36	0/2323	0.64	1/3144 (0.0%)
1	B	0.34	0/2199	0.60	0/2978
1	C	0.36	0/2323	0.64	0/3144
1	D	0.37	0/2214	0.62	0/2998
All	All	0.36	0/9059	0.63	1/12264 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ILE	N-CA-C	-5.12	97.19	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	2293	0	2381	94	0
1	B	2172	0	2252	98	0
1	C	2293	0	2381	91	0
1	D	2187	0	2265	101	0
2	A	135	0	0	19	0
2	B	78	0	0	9	0
2	C	115	0	0	11	0
2	D	122	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9395	0	9279	371	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 20.

The worst 5 of 371 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:86:THR:HB	1:A:89:ASP:HB2	1.32	1.07
1:B:90:LEU:HA	1:B:93:LYS:HD3	1.48	0.95
1:C:254:GLU:H	1:C:256:GLN:HE22	1.02	0.94
1:D:121:LEU:HD13	1:D:143:ALA:HB2	1.47	0.92
1:D:220:LYS:HG2	1:D:221:GLN:HE21	1.37	0.89

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	303/310 (98%)	274 (90%)	25 (8%)	4 (1%)	14	25
1	B	286/310 (92%)	261 (91%)	18 (6%)	7 (2%)	7	11
1	C	303/310 (98%)	277 (91%)	23 (8%)	3 (1%)	18	32
1	D	288/310 (93%)	265 (92%)	22 (8%)	1 (0%)	44	66
All	All	1180/1240 (95%)	1077 (91%)	88 (8%)	15 (1%)	14	25

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	285	GLN
1	A	80	PRO

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Mol	Chain	Res	Type
1	B	143	ALA
1	B	225	PHE
1	C	121	LEU

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	251/255 (98%)	245 (98%)	6 (2%)	54	80
1	B	237/255 (93%)	229 (97%)	8 (3%)	42	69
1	C	251/255 (98%)	239 (95%)	12 (5%)	30	53
1	D	239/255 (94%)	226 (95%)	13 (5%)	26	47
All	All	978/1020 (96%)	939 (96%)	39 (4%)	36	62

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	83	PRO
1	C	223	SER
1	D	270	LEU
1	C	100	GLU
1	C	105	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	111	ASN
1	C	301	ASN
1	D	282	ASN
1	C	126	HIS
1	C	256	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](#)

There are no ligands in this entry.

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	305/310 (98%)	-0.29	3 (0%) 82 83	7, 24, 49, 71	0
1	B	290/310 (93%)	-0.11	10 (3%) 46 48	10, 32, 53, 91	0
1	C	305/310 (98%)	-0.26	4 (1%) 77 78	7, 23, 51, 76	0
1	D	292/310 (94%)	-0.22	6 (2%) 64 66	7, 24, 50, 95	0
All	All	1192/1240 (96%)	-0.22	23 (1%) 67 69	7, 25, 52, 95	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	ILE	5.7
1	B	298	VAL	3.8
1	C	84	GLY	3.2
1	C	302	CYS	3.2
1	A	78	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.