



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:28 AM GMT

PDB ID : 2HAE
Title : Crystal structure of a putative malic enzyme (malate oxidoreductase)
Authors : Seetharaman, J.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-06-12
Resolution : 3.13 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

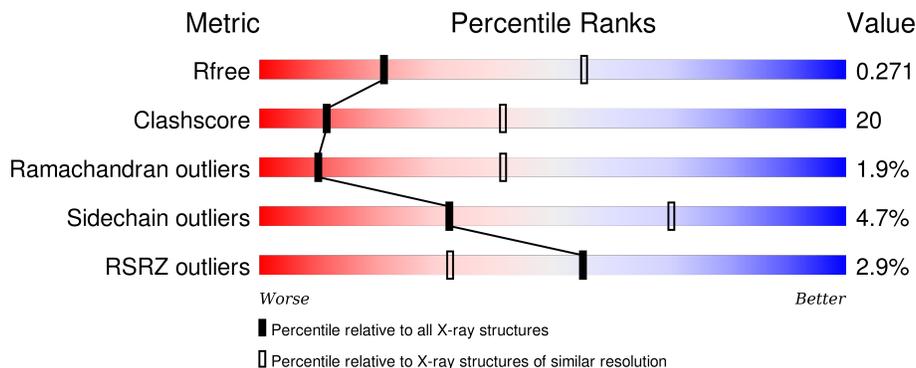
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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}	91344	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)

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	386	 66% 28% . .
1	B	386	 65% 30% . .
1	C	386	 60% 34% . .
1	D	386	 56% 37% . . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11756 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 oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	373	2860	1826	483	540	11	0	0	0
1	B	373	2860	1826	483	540	11	0	0	0
1	C	373	2860	1826	483	540	11	0	0	0
1	D	373	2860	1826	483	540	11	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	CLONING ARTIFACT	UNP Q9WZ12
A	0	SER	-	CLONING ARTIFACT	UNP Q9WZ12
A	1	LEU	-	CLONING ARTIFACT	UNP Q9WZ12
A	6	LEU	ILE	SEE REMARK 999	UNP Q9WZ12
A	377	GLU	-	CLONING ARTIFACT	UNP Q9WZ12
A	378	GLY	-	CLONING ARTIFACT	UNP Q9WZ12
A	379	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
A	380	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
A	381	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
A	382	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
A	383	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
A	384	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
B	-1	MET	-	CLONING ARTIFACT	UNP Q9WZ12
B	0	SER	-	CLONING ARTIFACT	UNP Q9WZ12
B	1	LEU	-	CLONING ARTIFACT	UNP Q9WZ12
B	6	LEU	ILE	SEE REMARK 999	UNP Q9WZ12
B	377	GLU	-	CLONING ARTIFACT	UNP Q9WZ12
B	378	GLY	-	CLONING ARTIFACT	UNP Q9WZ12
B	379	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
B	380	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
B	381	HIS	-	CLONING ARTIFACT	UNP Q9WZ12

Continued on next page...

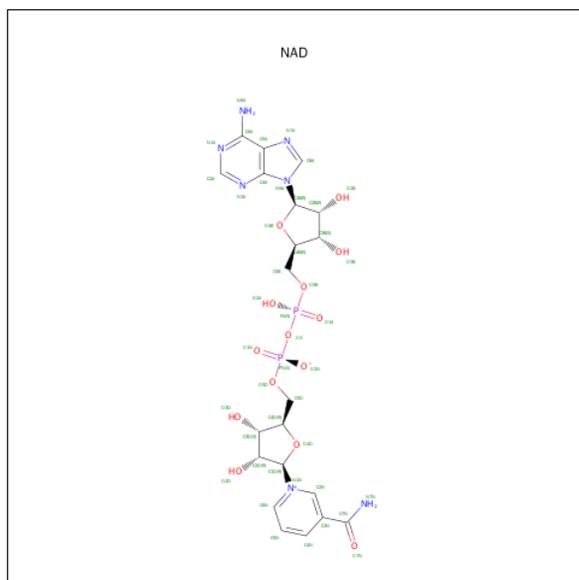
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	382	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
B	383	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
B	384	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
C	-1	MET	-	CLONING ARTIFACT	UNP Q9WZ12
C	0	SER	-	CLONING ARTIFACT	UNP Q9WZ12
C	1	LEU	-	CLONING ARTIFACT	UNP Q9WZ12
C	6	LEU	ILE	SEE REMARK 999	UNP Q9WZ12
C	377	GLU	-	CLONING ARTIFACT	UNP Q9WZ12
C	378	GLY	-	CLONING ARTIFACT	UNP Q9WZ12
C	379	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
C	380	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
C	381	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
C	382	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
C	383	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
C	384	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
D	-1	MET	-	CLONING ARTIFACT	UNP Q9WZ12
D	0	SER	-	CLONING ARTIFACT	UNP Q9WZ12
D	1	LEU	-	CLONING ARTIFACT	UNP Q9WZ12
D	6	LEU	ILE	SEE REMARK 999	UNP Q9WZ12
D	377	GLU	-	CLONING ARTIFACT	UNP Q9WZ12
D	378	GLY	-	CLONING ARTIFACT	UNP Q9WZ12
D	379	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
D	380	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
D	381	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
D	382	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
D	383	HIS	-	CLONING ARTIFACT	UNP Q9WZ12
D	384	HIS	-	CLONING ARTIFACT	UNP Q9WZ12

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	C	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total 44	O 44	0	0
4	B	41	Total 41	O 41	0	0
4	C	46	Total 46	O 46	0	0
4	D	52	Total 52	O 52	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	145.80Å 145.80Å 159.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.13 49.47 – 3.13	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.13) 94.9 (49.47-3.13)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.282 0.236 , 0.271	Depositor DCC
R_{free} test set	2425 reflections (8.16%)	DCC
Wilson B-factor (Å ²)	72.4	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.5	EDS
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 33596 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11756	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, NAD

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	0.47	0/2910	0.65	0/3942
1	B	0.47	0/2910	0.65	0/3942
1	C	0.48	0/2910	0.66	0/3942
1	D	0.49	0/2910	0.66	3/3942 (0.1%)
All	All	0.48	0/11640	0.65	3/15768 (0.0%)

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	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	155	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	130	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	154	ASP	CB-CG-OD2	5.23	123.00	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	316	LEU	Peptide

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	2860	0	2920	116	0
1	B	2860	0	2920	125	0
1	C	2860	0	2920	127	0
1	D	2860	0	2920	158	0
2	D	1	0	0	0	0
3	A	44	0	26	10	0
3	B	44	0	26	13	0
3	C	44	0	26	12	0
4	A	44	0	0	12	0
4	B	41	0	0	16	0
4	C	46	0	0	18	0
4	D	52	0	0	23	0
All	All	11756	0	11758	478	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 478 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)
3:A:501:NAD:H6N	1:B:283:ASN:HD22	1.13	1.11
1:B:32:TYR:OH	1:D:87:LYS:HE3	1.58	1.01
1:D:15:ARG:HG2	1:D:15:ARG:HH11	1.28	0.94
1:A:159:THR:CG2	3:B:501:NAD:H72N	1.79	0.94
3:A:501:NAD:C6N	1:B:283:ASN:HD22	1.82	0.92

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	369/386 (96%)	319 (86%)	43 (12%)	7 (2%)	10	41
1	B	369/386 (96%)	318 (86%)	47 (13%)	4 (1%)	17	56
1	C	369/386 (96%)	322 (87%)	39 (11%)	8 (2%)	8	37
1	D	369/386 (96%)	314 (85%)	46 (12%)	9 (2%)	7	35
All	All	1476/1544 (96%)	1273 (86%)	175 (12%)	28 (2%)	10	41

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	LEU
1	B	225	LEU
1	C	225	LEU
1	C	273	SER
1	D	225	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	309/321 (96%)	294 (95%)	15 (5%)	31	69
1	B	309/321 (96%)	295 (96%)	14 (4%)	34	71
1	C	309/321 (96%)	296 (96%)	13 (4%)	36	73
1	D	309/321 (96%)	293 (95%)	16 (5%)	29	65
All	All	1236/1284 (96%)	1178 (95%)	58 (5%)	32	70

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	314	ASN
1	C	127	ASN
1	D	274	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	335	ASN
1	C	6	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	148	ASN
1	C	262	ASN
1	D	308	HIS
1	C	186	ASN
1	A	335	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	A	501	-	38,48,48	1.90	7 (18%)	47,73,73	2.75	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	B	501	-	38,48,48	1.89	6 (15%)	47,73,73	2.71	14 (29%)
3	NAD	C	501	-	38,48,48	1.89	7 (18%)	47,73,73	2.74	12 (25%)

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
3	NAD	A	501	-	-	0/22/62/62	0/5/5/5
3	NAD	B	501	-	-	0/22/62/62	0/5/5/5
3	NAD	C	501	-	-	0/22/62/62	0/5/5/5

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NAD	C3N-C7N	-2.21	1.47	1.50
3	B	501	NAD	C3N-C7N	-2.12	1.47	1.50
3	A	501	NAD	C2N-C3N	2.08	1.42	1.39
3	A	501	NAD	C6N-N1N	2.09	1.41	1.35
3	B	501	NAD	C6N-N1N	2.16	1.41	1.35

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAD	N3A-C2A-N1A	-10.60	120.78	128.89
3	B	501	NAD	N3A-C2A-N1A	-10.53	120.83	128.89
3	C	501	NAD	N3A-C2A-N1A	-10.47	120.88	128.89
3	B	501	NAD	O3-PN-O5D	-8.89	79.36	102.94
3	A	501	NAD	O3-PN-O5D	-8.85	79.47	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	NAD	10	0
3	B	501	NAD	13	0
3	C	501	NAD	12	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, 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	373/386 (96%)	-0.11	2 (0%) 91 84	24, 51, 66, 75	2 (0%)
1	B	373/386 (96%)	-0.11	2 (0%) 91 84	24, 52, 66, 75	2 (0%)
1	C	373/386 (96%)	0.22	28 (7%) 17 6	23, 54, 67, 77	2 (0%)
1	D	373/386 (96%)	0.03	11 (2%) 55 32	23, 54, 67, 76	2 (0%)
All	All	1492/1544 (96%)	0.00	43 (2%) 55 32	23, 53, 67, 77	8 (0%)

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	269	ILE	4.0
1	C	297	GLY	3.9
1	C	298	ALA	3.9
1	C	270	LYS	3.7
1	C	299	PHE	3.6

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NAD	C	501	44/44	0.88	0.35	1.11	54,56,65,66	0
3	NAD	B	501	44/44	0.88	0.26	0.81	52,56,64,68	0
3	NAD	A	501	44/44	0.88	0.26	0.49	53,55,64,67	0
2	ZN	D	800	1/1	0.93	0.10	-5.10	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.