



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2017 – 09:25 PM EDT

PDB ID : 5L46  
Title : Crystal structure of human dimethylglycine-dehydrogenase  
Authors : Hromic, A.; Pavkov-Keller, T.; Gruber, K.  
Deposited on : unknown  
Resolution : 3.09 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
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)	:	rb-20029824

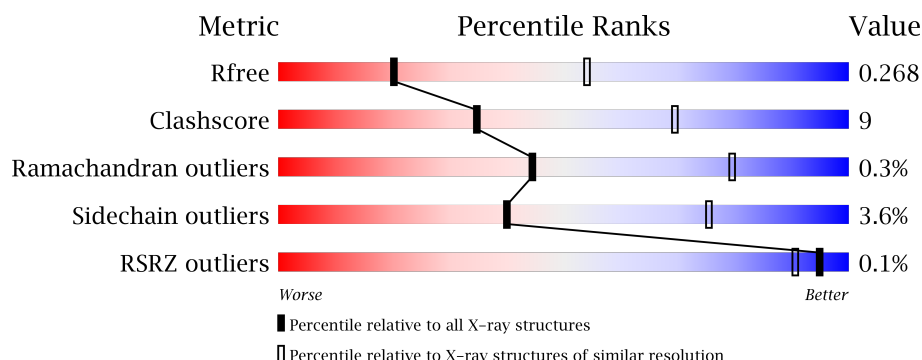
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 3.09 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	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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  $\geq 3$ , 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	841	
1	B	841	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12894 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.

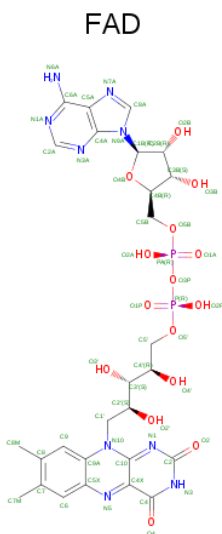
- Molecule 1 is a protein called Dimethylglycine dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	809	Total	C	N	O	S	0	0	0
			6398	4099	1090	1186	23			
1	B	808	Total	C	N	O	S	0	0	0
			6384	4088	1088	1185	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP Q9UI17
A	279	PRO	SER	conflict	UNP Q9UI17
A	867	ARG	-	expression tag	UNP Q9UI17
A	868	PRO	-	expression tag	UNP Q9UI17
B	28	MET	-	initiating methionine	UNP Q9UI17
B	279	PRO	SER	conflict	UNP Q9UI17
B	867	ARG	-	expression tag	UNP Q9UI17
B	868	PRO	-	expression tag	UNP Q9UI17

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

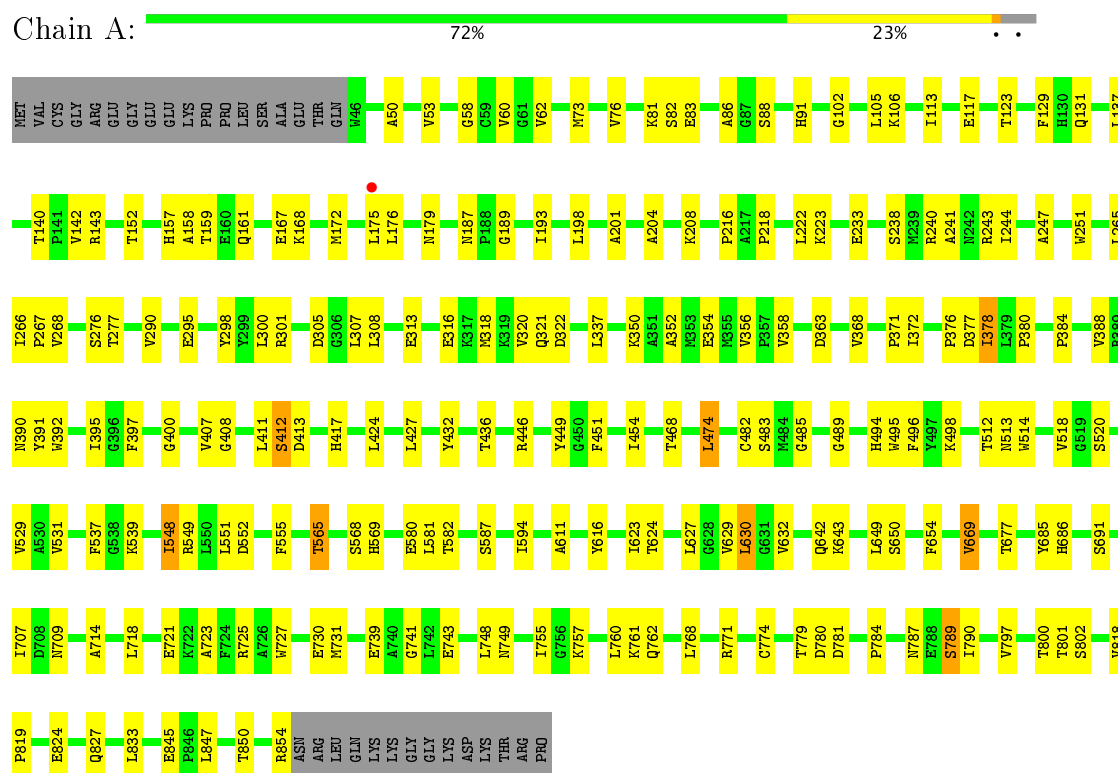
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	2	Total O 2 2	0	0

### 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 ( $RSRZ > 2$ ). 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: Dimethylglycine dehydrogenase, mitochondrial



- Molecule 1: Dimethylglycine dehydrogenase, mitochondrial



V796	RG88	V562	D423
V797	D689	T565	L424
T801	S691	H566	Y432
S802	F710	I567	
	N716	S568	T436
L813			
A814	R719	T572	R446
F815	L720	P573	E447
V818	E721	K574	S448
P819	K722	Y578	Y449
			G450
L822	R725	L581	F451
S823	A726	L582	M452
E824	E727	S587	M453
		P588	L454
Q827	W730	I594	Y457
L833	N732		
L834	C733	R605	R462
G835			
K836	L738	V612	R466
N837	E739	K621	C482
I842	F745	T624	G485
	V746		F486
E845		L627	H487
P846	N749		E491
L847		L630	Q492
V848	Q758		P493
L849	A759	R638	A494
T850	L760		W495
E851	K761	K643	F496
P852	Q762	L644	
T853	A765	S650	P507
R854			
ASN	L768	F654	R511
LEU	K769		T512
GLN		L657	N513
LYS	L772	Q658	W514
LYS	L775	T659	
GLY	L776	K660	Q524
GLY	L777		
LYS		V684	E530
ASP		I687	T532
LYS	D780	P688	F637
THR	D781	V689	G538
ARG			K539
	P784	I672	F540
			N541
	N787	W632	I542
	I790		
	N793	V685	L551
	G794	H686	
	W795	P687	P555

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.38Å 119.87Å 86.47Å 90.00° 92.58° 90.00°	Depositor
Resolution (Å)	58.65 – 3.09 58.65 – 3.09	Depositor EDS
% Data completeness (in resolution range)	97.7 (58.65-3.09) 97.7 (58.65-3.09)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.8.4 _1496	Depositor
R, $R_{free}$	0.179 , 0.269 0.181 , 0.268	Depositor DCC
$R_{free}$ test set	1524 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.003 for l,k,-h 0.068 for h,-k,-l 0.030 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

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	0.49	1/6558 (0.0%)	0.66	0/8895
1	B	0.50	0/6542	0.64	1/8872 (0.0%)
All	All	0.50	1/13100 (0.0%)	0.65	1/17767 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	774	CYS	CB-SG	-5.00	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	813	LEU	CA-CB-CG	5.69	128.39	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	6398	0	6352	115	0
1	B	6384	0	6342	128	0
2	A	53	0	30	6	0
2	B	53	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	0	0	0
3	B	2	0	0	0	0
All	All	12894	0	12754	241	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 9.

The worst 5 of 241 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:290:VAL:HG13	1:B:301:ARG:HB3	1.54	0.90
1:B:487:HIS:CD2	1:B:492:GLN:HE21	2.01	0.78
1:A:290:VAL:HG13	1:A:301:ARG:HB3	1.66	0.76
1:A:755:ILE:HD11	1:B:793:ASN:HD21	1.53	0.74
1:B:115:LEU:HA	1:B:118:LYS:HE2	1.71	0.72

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	807/841 (96%)	765 (95%)	39 (5%)	3 (0%)	38	75
1	B	806/841 (96%)	756 (94%)	48 (6%)	2 (0%)	51	84
All	All	1613/1682 (96%)	1521 (94%)	87 (5%)	5 (0%)	44	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	ILE
1	B	378	ILE

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Mol	Chain	Res	Type
1	A	537	PHE
1	B	102	GLY
1	A	102	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	682/709 (96%)	657 (96%)	25 (4%)	39	75
1	B	681/709 (96%)	657 (96%)	24 (4%)	41	76
All	All	1363/1418 (96%)	1314 (96%)	49 (4%)	40	75

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	779	THR
1	B	163	LEU
1	B	801	THR
1	A	801	THR
1	B	254	GLU

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	452	ASN
1	A	494	HIS
1	B	487	HIS
1	B	793	ASN

### 5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

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$
2	FAD	A	901	1	51,58,58	1.42	8 (15%)	54,89,89	3.24	12 (22%)
2	FAD	B	901	1	51,58,58	1.45	7 (13%)	54,89,89	2.38	14 (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
2	FAD	A	901	1	-	0/28/50/50	0/6/6/6
2	FAD	B	901	1	-	0/28/50/50	0/6/6/6

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	FAD	C2-N3	-2.20	1.33	1.38
2	A	901	FAD	O4B-C1B	2.23	1.44	1.41
2	B	901	FAD	O4B-C1B	2.26	1.44	1.41
2	A	901	FAD	C9A-N10	2.46	1.42	1.38
2	A	901	FAD	C5A-C4A	2.49	1.46	1.40

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	FAD	C1'-N10-C9A	-9.51	109.63	118.35
2	A	901	FAD	N3A-C2A-N1A	-6.64	123.07	128.86
2	B	901	FAD	N3A-C2A-N1A	-5.59	123.99	128.86
2	B	901	FAD	C4B-O4B-C1B	-4.29	105.20	109.77
2	B	901	FAD	C4X-C4-N3	-4.20	117.51	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	FAD	6	0
2	B	901	FAD	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	809/841 (96%)	-0.34	1 (0%) 95 90	7, 36, 61, 98	0
1	B	808/841 (96%)	-0.36	0 100 100	10, 36, 62, 105	0
All	All	1617/1682 (96%)	-0.35	1 (0%) 95 90	7, 36, 62, 105	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	LEU	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. 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	FAD	B	901	53/53	0.95	0.17	-0.36	34,34,34,34	0
2	FAD	A	901	53/53	0.95	0.17	-0.42	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.