



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:23 pm GMT

PDB ID : 4PVC  
Title : Crystal structure of yeast methylglyoxal/ isovaleraldehyde reductase Gre2  
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Deposited on : 2014-03-17  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
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

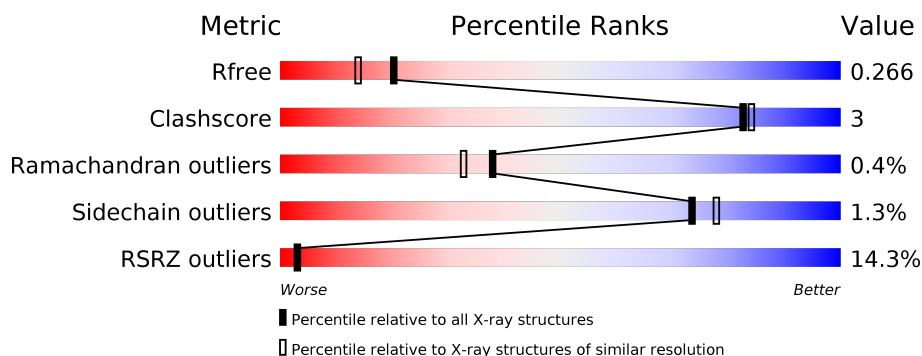
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	342	<div> <div>10%</div> <div>93%</div> <div>6%</div> </div>
1	B	342	<div> <div>18%</div> <div>94%</div> <div>6%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5726 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 NADPH-dependent methylglyoxal reductase GRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2690	1714	452	514	10			
1	B	342	Total	C	N	O	S	0	0	0
			2690	1714	452	514	10			

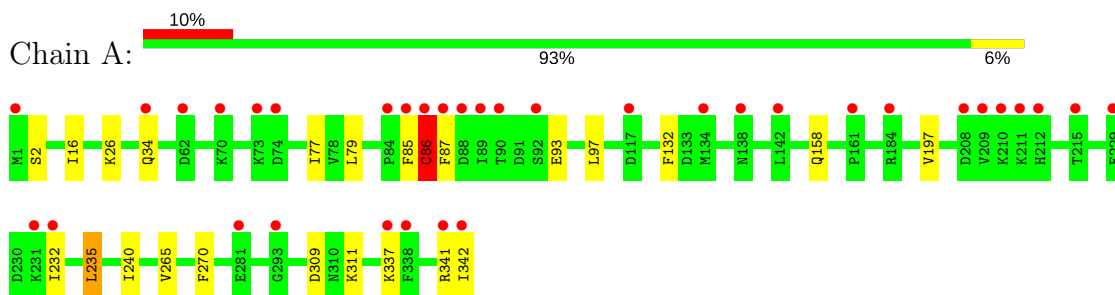
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	185	Total	O	0	0
			185	185		
2	B	161	Total	O	0	0
			161	161		

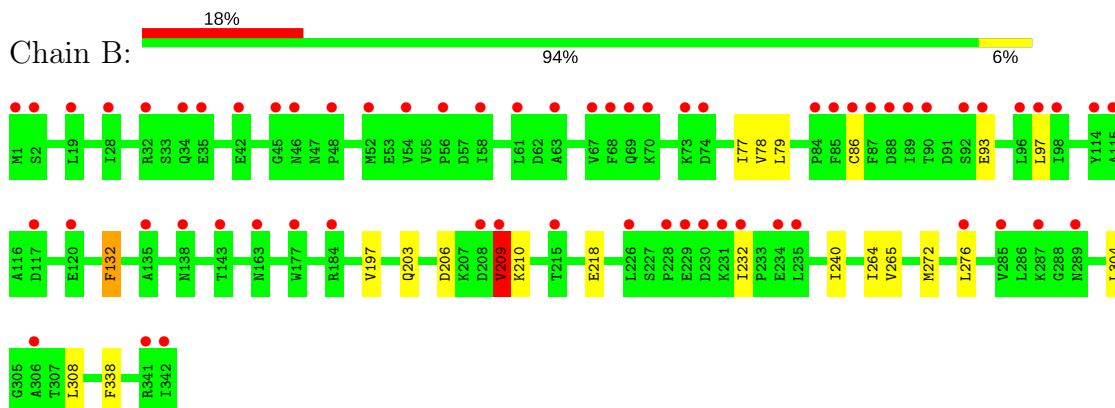
### 3 Residue-property plots [i](#)

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: NADPH-dependent methylglyoxal reductase GRE2



- Molecule 1: NADPH-dependent methylglyoxal reductase GRE2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.72Å 97.84Å 139.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 34.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.00) 98.8 (34.75-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.77 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.224 , 0.266 0.224 , 0.266	Depositor DCC
$R_{free}$ test set	2281 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5726	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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](#)

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	0.42	0/2745	0.53	0/3705
1	B	0.41	1/2745 (0.0%)	0.50	0/3705
All	All	0.42	1/5490 (0.0%)	0.51	0/7410

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	VAL	CB-CG2	-5.77	1.40	1.52

There are no bond angle outliers.

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	2690	0	2679	16	0
1	B	2690	0	2679	18	0
2	A	185	0	0	1	0
2	B	161	0	0	2	0
All	All	5726	0	5358	31	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 3.

All (31) 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:206:ASP:O	1:B:209:VAL:HG13	1.85	0.76
1:A:86:CYS:SG	1:A:87:PHE:N	2.63	0.72
1:B:77:ILE:HG22	1:B:79:LEU:CD1	2.20	0.71
1:A:85:PHE:O	1:A:86:CYS:HB3	1.95	0.65
1:B:77:ILE:HG22	1:B:79:LEU:HD11	1.79	0.64
1:A:309:ASP:OD1	1:A:311:LYS:HG2	2.01	0.60
1:A:86:CYS:HB2	1:B:86:CYS:SG	2.43	0.58
1:B:132:PHE:HB2	2:B:561:HOH:O	2.05	0.57
1:B:79:LEU:HD12	1:B:79:LEU:N	2.22	0.54
1:B:78:VAL:C	1:B:79:LEU:HD12	2.30	0.52
1:B:210:LYS:HB2	1:B:338:PHE:CZ	2.45	0.52
1:B:79:LEU:N	1:B:79:LEU:CD1	2.75	0.50
1:B:203:GLN:NE2	2:B:551:HOH:O	2.44	0.49
1:A:86:CYS:SG	1:B:86:CYS:HB2	2.52	0.49
1:B:77:ILE:CG2	1:B:79:LEU:HD11	2.42	0.49
1:A:235:LEU:HD21	1:A:270:PHE:CE1	2.47	0.49
1:A:235:LEU:HD23	1:A:235:LEU:O	2.14	0.48
1:B:232:ILE:HD12	1:B:276:LEU:HD11	1.95	0.48
1:A:235:LEU:HD23	1:A:235:LEU:C	2.33	0.48
1:B:93:GLU:HA	1:B:97:LEU:HB2	1.96	0.47
1:A:16:ILE:HG21	1:A:79:LEU:HD23	1.97	0.46
1:A:337:LYS:HG2	1:A:342:ILE:HG22	1.97	0.46
1:B:264:ILE:HG21	1:B:308:LEU:HD21	1.98	0.46
1:B:272:MET:HA	1:B:272:MET:CE	2.46	0.45
1:A:240:ILE:HG12	1:A:265:VAL:HG12	1.99	0.45
1:A:77:ILE:HG22	1:A:79:LEU:CD1	2.47	0.45
1:B:240:ILE:HG12	1:B:265:VAL:HG12	2.00	0.44
1:A:93:GLU:HA	1:A:97:LEU:HB2	1.99	0.44
1:A:34:GLN:NE2	2:A:576:HOH:O	2.50	0.44
1:A:2:SER:HA	1:A:26:LYS:O	2.19	0.42
1:A:158:GLN:O	1:B:218:GLU:HG2	2.21	0.41

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	340/342 (99%)	332 (98%)	6 (2%)	2 (1%)	28	21
1	B	340/342 (99%)	336 (99%)	3 (1%)	1 (0%)	44	40
All	All	680/684 (99%)	668 (98%)	9 (1%)	3 (0%)	38	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	VAL
1	B	197	VAL
1	A	86	CYS

### 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	297/297 (100%)	292 (98%)	5 (2%)	66	70
1	B	297/297 (100%)	294 (99%)	3 (1%)	80	84
All	All	594/594 (100%)	586 (99%)	8 (1%)	73	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	CYS
1	A	132	PHE
1	A	232	ILE
1	A	235	LEU
1	A	341	ARG
1	B	132	PHE
1	B	209	VAL
1	B	304	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	301	HIS

### 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

### 6.1 Protein, DNA and RNA chains

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	342/342 (100%)	0.78	35 (10%) <b>7</b> <b>8</b>	35, 52, 70, 84	0
1	B	342/342 (100%)	1.09	63 (18%) <b>1</b> <b>1</b>	36, 59, 80, 91	0
All	All	684/684 (100%)	0.93	98 (14%) <b>3</b> <b>3</b>	35, 55, 78, 91	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	CYS	6.9
1	A	1	MET	6.7
1	B	85	PHE	6.3
1	B	74	ASP	5.5
1	B	342	ILE	5.4
1	B	117	ASP	5.0
1	B	35	GLU	4.9
1	B	208	ASP	4.8
1	A	342	ILE	4.8
1	A	231	LYS	4.7
1	A	90	THR	4.4
1	A	208	ASP	4.4
1	A	85	PHE	4.4
1	A	229	GLU	4.3
1	B	1	MET	4.2
1	B	90	THR	4.2
1	B	215	THR	4.0
1	A	212	HIS	3.9
1	B	234	GLU	3.8
1	A	209	VAL	3.8
1	A	337	LYS	3.8
1	B	163	ASN	3.8
1	B	88	ASP	3.8
1	B	86	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	68	PHE	3.7
1	B	229	GLU	3.7
1	A	73	LYS	3.6
1	B	87	PHE	3.5
1	B	232	ILE	3.4
1	A	232	ILE	3.4
1	A	89	ILE	3.3
1	A	338	PHE	3.3
1	B	114	TYR	3.3
1	B	73	LYS	3.2
1	B	48	PRO	3.1
1	A	210	LYS	3.1
1	A	74	ASP	3.1
1	A	117	ASP	3.0
1	B	42	GLU	3.0
1	B	32	ARG	3.0
1	B	84	PRO	2.9
1	A	138	ASN	2.9
1	B	231	LYS	2.9
1	B	70	LYS	2.9
1	B	89	ILE	2.8
1	B	92	SER	2.8
1	B	45	GLY	2.8
1	B	97	LEU	2.8
1	B	58	ILE	2.8
1	A	341	ARG	2.8
1	A	84	PRO	2.7
1	B	46	ASN	2.7
1	A	92	SER	2.7
1	B	228	PRO	2.7
1	B	61	LEU	2.6
1	B	67	VAL	2.6
1	A	184	ARG	2.6
1	B	98	ILE	2.6
1	B	287	LYS	2.6
1	B	93	GLU	2.6
1	B	184	ARG	2.6
1	B	96	LEU	2.6
1	B	306	ALA	2.5
1	B	138	ASN	2.5
1	B	63	ALA	2.5
1	B	289	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	161	PRO	2.4
1	A	87	PHE	2.4
1	B	120	GLU	2.4
1	B	2	SER	2.3
1	A	70	LYS	2.3
1	B	235	LEU	2.3
1	B	69	GLN	2.3
1	B	230	ASP	2.3
1	A	215	THR	2.3
1	A	142	LEU	2.2
1	B	143	THR	2.2
1	A	281	GLU	2.2
1	B	285	VAL	2.2
1	B	19	LEU	2.1
1	B	52	MET	2.1
1	A	88	ASP	2.1
1	A	134	MET	2.1
1	B	56	PRO	2.1
1	B	341	ARG	2.1
1	B	226	LEU	2.1
1	A	62	ASP	2.1
1	A	34	GLN	2.1
1	B	115	ALA	2.1
1	B	135	ALA	2.0
1	B	209	VAL	2.0
1	A	293	GLY	2.0
1	A	211	LYS	2.0
1	B	28	ILE	2.0
1	B	276	LEU	2.0
1	B	54	VAL	2.0
1	B	34	GLN	2.0
1	B	177	TRP	2.0

## 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.