



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:50 PM GMT

PDB ID : 1CRW  
Title : CRYSTAL STRUCTURE OF APO-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE FROM PALINURUS VERSICOLOR AT 2.0A RESOLUTION  
Authors : Shen, Y.; Li, J.; Song, S.; Lin, Z.  
Deposited on : 1999-08-16  
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.

---

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

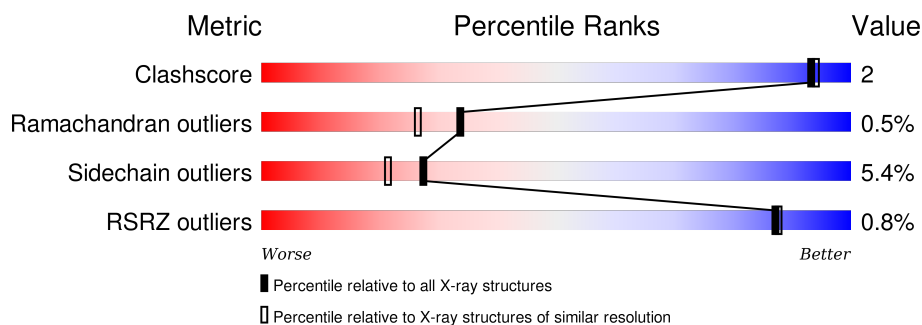
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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	G	333	<div> <div></div> <div>88% 11% .</div> </div>
1	R	333	<div> <div></div> <div>86% 12% .</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5337 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 D-GLYCERALDEHYDE-3-PHOSPHATE-DEHYDROGEN ASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	333	Total	C	N	O	S	0	0	0
			2506	1589	421	480	16			
1	R	333	Total	C	N	O	S	0	0	0
			2506	1589	421	480	16			

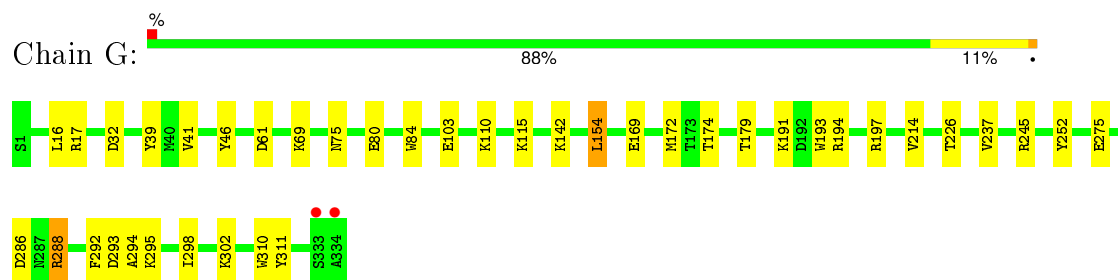
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	194	Total	O	0	0
			194	194		
2	R	131	Total	O	0	0
			131	131		

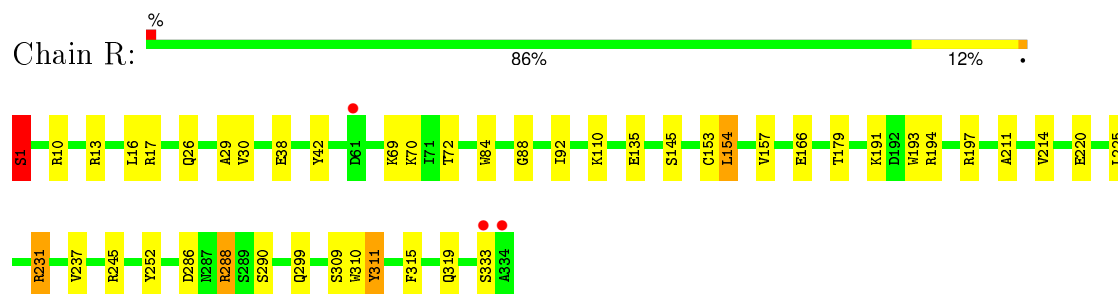
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: D-GLYCERALDEHYDE-3-PHOSPHATE-DEHYDROGENASE



- Molecule 1: D-GLYCERALDEHYDE-3-PHOSPHATE-DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.45Å 99.84Å 80.79Å 90.00° 115.14° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00 6.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	0.7 (6.00-2.00) 57.8 (6.00-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.165 , 0.226 0.161 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	10.4	Xtriage
Anisotropy	0.819	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 84.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 47932 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5337	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	G	0.81	0/2551	1.46	28/3446 (0.8%)
1	R	0.77	0/2551	1.45	23/3446 (0.7%)
All	All	0.79	0/5102	1.46	51/6892 (0.7%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	288	ARG	NE-CZ-NH1	13.96	127.28	120.30
1	G	288	ARG	NE-CZ-NH2	-11.32	114.64	120.30
1	G	197	ARG	NE-CZ-NH2	9.62	125.11	120.30
1	R	17	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	G	310	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	G	310	TRP	CE2-CD2-CG	-8.88	100.20	107.30
1	R	310	TRP	CD1-CG-CD2	8.83	113.36	106.30
1	R	288	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	R	84	TRP	CD1-CG-CD2	8.59	113.17	106.30
1	G	17	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	R	84	TRP	CE2-CD2-CG	-7.68	101.16	107.30
1	R	197	ARG	NE-CZ-NH2	7.63	124.12	120.30
1	G	84	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	G	197	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	G	252	TYR	CB-CG-CD2	-7.35	116.59	121.00
1	R	194	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	R	252	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	R	310	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	R	193	TRP	CD1-CG-CD2	7.14	112.01	106.30
1	G	193	TRP	CD1-CG-CD2	6.81	111.75	106.30
1	G	84	TRP	CE2-CD2-CG	-6.77	101.89	107.30
1	G	84	TRP	CG-CD2-CE3	6.66	139.89	133.90
1	R	197	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	G	193	TRP	CE2-CD2-CG	-6.14	102.39	107.30
1	G	46	TYR	CB-CG-CD2	-5.98	117.41	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	84	TRP	CB-CG-CD1	-5.96	119.25	127.00
1	G	245	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	R	288	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	G	84	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	R	310	TRP	CG-CD1-NE1	-5.75	104.35	110.10
1	G	169	GLU	CA-C-N	5.70	127.60	116.20
1	R	13	ARG	N-CA-CB	-5.62	100.48	110.60
1	R	245	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	R	193	TRP	CE2-CD2-CG	-5.59	102.83	107.30
1	G	80	GLU	CA-CB-CG	5.58	125.68	113.40
1	G	310	TRP	CG-CD2-CE3	5.57	138.92	133.90
1	R	1	SER	N-CA-CB	-5.54	102.19	110.50
1	R	84	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	R	299	GLN	CA-CB-CG	-5.38	101.56	113.40
1	G	39	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	R	42	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	R	84	TRP	CB-CG-CD1	-5.31	120.10	127.00
1	G	310	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	G	17	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	G	293	ASP	CB-CG-OD2	5.20	122.98	118.30
1	G	226	THR	CA-CB-CG2	5.15	119.61	112.40
1	R	311	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	G	194	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	G	226	THR	CA-CB-OG1	-5.07	98.34	109.00
1	G	41	VAL	CG1-CB-CG2	-5.06	102.81	110.90
1	R	30	VAL	CG1-CB-CG2	-5.04	102.84	110.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	G	2506	0	2529	8	0
1	R	2506	0	2529	11	0
2	G	194	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	131	0	0	2	0
All	All	5337	0	5058	19	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 2.

All (19) 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:G:154:LEU:HD13	1:G:214:VAL:HG21	1.68	0.74
1:R:154:LEU:HD13	1:R:214:VAL:HG21	1.71	0.71
1:G:286:ASP:OD2	1:G:288:ARG:HD3	2.09	0.52
1:R:1:SER:N	1:R:26:GLN:HB3	2.26	0.50
1:R:211:ALA:HB1	1:R:225:LEU:HB3	1.93	0.50
1:R:286:ASP:OD2	1:R:288:ARG:HD3	2.11	0.48
1:R:220:GLU:HB2	2:R:421:HOH:O	2.14	0.48
1:R:69:LYS:HD2	1:R:69:LYS:H	1.82	0.44
1:R:29:ALA:HA	1:R:72:THR:O	2.17	0.44
1:R:110:LYS:HD3	1:R:110:LYS:HA	1.75	0.43
1:G:191:LYS:HD3	1:G:191:LYS:HA	1.86	0.42
1:G:32:ASP:O	1:G:75:ASN:HA	2.20	0.41
1:G:292:PHE:CE2	1:G:294:ALA:HA	2.56	0.41
1:R:179:THR:OG1	1:R:231:ARG:NH2	2.54	0.41
1:G:179:THR:HB	2:G:460:HOH:O	2.20	0.41
1:G:275:GLU:O	1:G:295:LYS:HD3	2.21	0.41
1:R:88:GLY:HA3	2:R:387:HOH:O	2.21	0.40
1:R:153:CYS:HA	1:R:290:SER:HB2	2.02	0.40
1:G:142:LYS:HE2	1:G:142:LYS:HB3	1.88	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	G	331/333 (99%)	319 (96%)	11 (3%)	1 (0%)	46	41
1	R	331/333 (99%)	319 (96%)	10 (3%)	2 (1%)	30	22
All	All	662/666 (99%)	638 (96%)	21 (3%)	3 (0%)	34	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	237	VAL
1	R	237	VAL
1	R	166	GLU

### 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	G	269/269 (100%)	257 (96%)	12 (4%)	34	29
1	R	269/269 (100%)	252 (94%)	17 (6%)	22	16
All	All	538/538 (100%)	509 (95%)	29 (5%)	27	21

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	16	LEU
1	G	61	ASP
1	G	69	LYS
1	G	103	GLU
1	G	110	LYS
1	G	115	LYS
1	G	154	LEU
1	G	172	MET
1	G	174	THR
1	G	298	ILE
1	G	302	LYS
1	G	311	TYR
1	R	1	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	R	10	ARG
1	R	16	LEU
1	R	38	GLU
1	R	70	LYS
1	R	92	ILE
1	R	135	GLU
1	R	145	SER
1	R	154	LEU
1	R	157	VAL
1	R	191	LYS
1	R	231	ARG
1	R	309	SER
1	R	311	TYR
1	R	315	PHE
1	R	319	GLN
1	R	333	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	268	GLN
1	R	81	ASN
1	R	164	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](#)

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	G	333/333 (100%)	-1.22	2 (0%) 90 90	6, 17, 35, 66	0
1	R	333/333 (100%)	-0.96	3 (0%) 85 86	8, 23, 51, 82	0
All	All	666/666 (100%)	-1.09	5 (0%) 87 88	6, 19, 48, 82	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	333	SER	5.0
1	R	334	ALA	3.6
1	G	333	SER	3.0
1	G	334	ALA	2.8
1	R	61	ASP	2.1

### 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.