



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 09:45 pm GMT

PDB ID : 1GQN  
Title : NATIVE 3-DEHYDROQUINASE FROM SALMONELLA TYPHI  
Authors : Lee, W.-H.; Perles, L.A.; Nagem, R.A.P.; Polikarpov, I.; Sawyer, L.  
Deposited on : 2001-11-26  
Resolution : 1.78 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

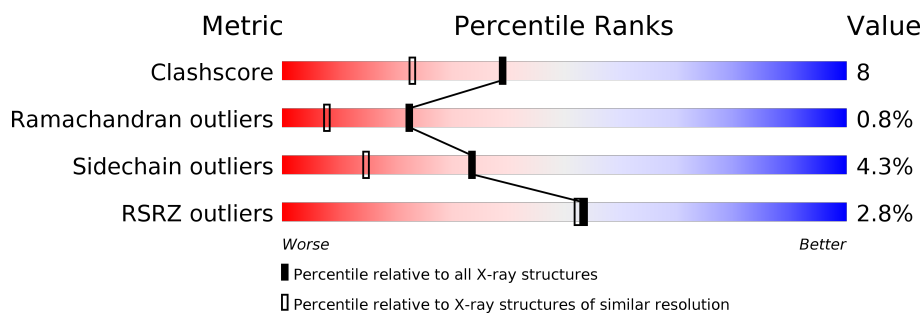
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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	252	<div> <div>3%</div> <div>76%</div> <div>19%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2115 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 3-DEHYDROQUINATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1934	1219	335	366	14			

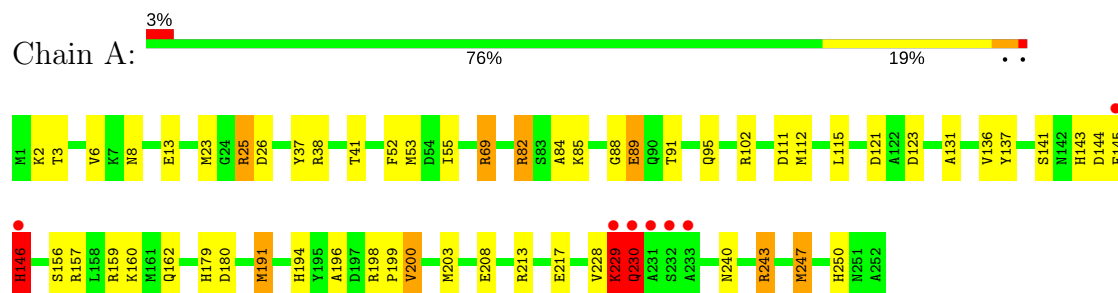
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	181	Total	O	0	0
			181	181		

### 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: 3-DEHYDROQUINATE DEHYDRATASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.78Å 112.33Å 42.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.75 – 1.78 11.75 – 1.78	Depositor EDS
% Data completeness (in resolution range)	97.2 (11.75-1.78) 97.2 (11.75-1.78)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.199 , 0.247 0.172 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2115	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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	0.89	4/1965 (0.2%)	1.82	42/2661 (1.6%)

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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	PRO	C-N	-6.37	1.19	1.34
1	A	200	VAL	C-N	-5.75	1.20	1.34
1	A	247	MET	C-N	-5.46	1.21	1.34
1	A	141	SER	CA-CB	5.37	1.61	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ARG	NE-CZ-NH1	-12.82	113.89	120.30
1	A	102	ARG	CD-NE-CZ	12.38	140.93	123.60
1	A	102	ARG	NE-CZ-NH2	11.38	125.99	120.30
1	A	198	ARG	NE-CZ-NH2	-11.25	114.67	120.30
1	A	199	PRO	C-N-CA	10.53	148.03	121.70
1	A	37	TYR	CB-CG-CD1	9.22	126.53	121.00
1	A	111	ASP	CB-CG-OD2	8.94	126.35	118.30
1	A	199	PRO	CA-C-N	8.30	135.45	117.20
1	A	38	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	191	MET	CA-CB-CG	7.47	126.00	113.30
1	A	38	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	199	PRO	O-C-N	-7.30	111.02	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	A	198	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	159	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	82	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	102	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	A	136	VAL	CA-CB-CG1	6.78	121.08	110.90
1	A	123	ASP	CB-CG-OD1	-6.54	112.41	118.30
1	A	180	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	A	131	ALA	O-C-N	-6.25	112.70	122.70
1	A	23	MET	CG-SD-CE	6.15	110.04	100.20
1	A	247	MET	CG-SD-CE	6.14	110.03	100.20
1	A	145	PHE	CB-CG-CD1	-6.03	116.58	120.80
1	A	69	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	A	121	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	136	VAL	CG1-CB-CG2	-5.65	101.86	110.90
1	A	131	ALA	CA-C-O	5.61	131.89	120.10
1	A	146	HIS	CB-CA-C	-5.60	99.19	110.40
1	A	115	LEU	O-C-N	5.49	131.48	122.70
1	A	52	PHE	CB-CG-CD1	-5.39	117.02	120.80
1	A	25	ARG	CA-CB-CG	5.38	125.24	113.40
1	A	141	SER	N-CA-CB	-5.37	102.45	110.50
1	A	247	MET	O-C-N	-5.34	114.15	122.70
1	A	26	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	194	HIS	CB-CA-C	-5.18	100.04	110.40
1	A	243	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	89	GLU	N-CA-CB	-5.15	101.33	110.60
1	A	145	PHE	CA-CB-CG	-5.04	101.80	113.90
1	A	145	PHE	CB-CA-C	-5.01	100.37	110.40
1	A	157	ARG	CG-CD-NE	5.01	122.32	111.80
1	A	194	HIS	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	VAL	Mainchain

## 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	A	1934	0	1961	33	0
2	A	181	0	0	12	0
All	All	2115	0	1961	33	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 8.

All (33) 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:156:SER:OG	2:A:2117:HOH:O	1.87	0.91
1:A:162:GLN:HE22	1:A:196:ALA:HA	1.47	0.77
1:A:240:ASN:HD22	1:A:243:ARG:HH11	1.39	0.69
1:A:3:THR:HG21	1:A:13:GLU:HG3	1.75	0.68
1:A:240:ASN:ND2	1:A:243:ARG:HH11	1.92	0.67
1:A:240:ASN:HB2	2:A:2177:HOH:O	1.96	0.65
1:A:112:MET:HG2	1:A:137:TYR:HB2	1.78	0.65
1:A:217:GLU:OE2	1:A:250:HIS:HD2	1.80	0.64
1:A:89:GLU:O	2:A:2072:HOH:O	2.14	0.64
1:A:203:MET:HE3	2:A:2163:HOH:O	1.98	0.63
1:A:84:ALA:HB3	1:A:91:THR:HG22	1.81	0.62
1:A:146:HIS:HE1	2:A:2104:HOH:O	1.83	0.61
1:A:247:MET:SD	2:A:2071:HOH:O	2.56	0.60
1:A:146:HIS:CE1	2:A:2104:HOH:O	2.56	0.58
1:A:229:LYS:O	1:A:230:GLN:C	2.44	0.55
1:A:25:ARG:HB3	1:A:53:MET:HG2	1.91	0.53
1:A:41:THR:HB	1:A:243:ARG:NH1	2.24	0.53
1:A:179:HIS:HB3	2:A:2135:HOH:O	2.08	0.52
1:A:91:THR:HG23	2:A:2037:HOH:O	2.11	0.50
1:A:84:ALA:CB	1:A:91:THR:HG22	2.42	0.49
1:A:208:GLU:HB2	2:A:2151:HOH:O	2.14	0.47
1:A:144:ASP:OD1	1:A:146:HIS:ND1	2.47	0.46
1:A:228:VAL:O	1:A:230:GLN:NE2	2.49	0.45
1:A:8:ASN:ND2	2:A:2013:HOH:O	2.49	0.45
1:A:229:LYS:O	1:A:230:GLN:O	2.36	0.42
1:A:162:GLN:NE2	1:A:196:ALA:HA	2.24	0.42
1:A:213:ARG:HH11	1:A:213:ARG:HD3	1.66	0.42
1:A:228:VAL:O	1:A:229:LYS:O	2.39	0.41
1:A:229:LYS:HB3	1:A:230:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:NZ	2:A:2127:HOH:O	2.49	0.41
1:A:69:ARG:HD3	1:A:69:ARG:HA	1.87	0.40
1:A:82:ARG:CZ	1:A:143:HIS:CE1	3.04	0.40
1:A:82:ARG:O	1:A:88:GLY:HA3	2.20	0.40

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	250/252 (99%)	243 (97%)	5 (2%)	2 (1%)	22 8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	229	LYS

### 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	209/209 (100%)	200 (96%)	9 (4%)	33 15

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	6	VAL
1	A	55	ILE
1	A	85	LYS
1	A	95	GLN
1	A	146	HIS
1	A	191	MET
1	A	229	LYS
1	A	230	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	162	GLN
1	A	236	GLN
1	A	240	ASN
1	A	250	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 ⓘ

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	252/252 (100%)	-0.18	7 (2%) 53 52	13, 24, 42, 86	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	GLN	5.9
1	A	229	LYS	5.4
1	A	233	ALA	3.7
1	A	146	HIS	3.7
1	A	231	ALA	3.5
1	A	232	SER	3.5
1	A	145	PHE	2.9

### 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.