



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 30, 2023 – 06:05 PM EST

PDB ID : 8ETN  
Title : The X-ray Crystal Structure of Tri-Ketone Dioxygenase from Rice  
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Deposited on : 2022-10-17  
Resolution : 3.16 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

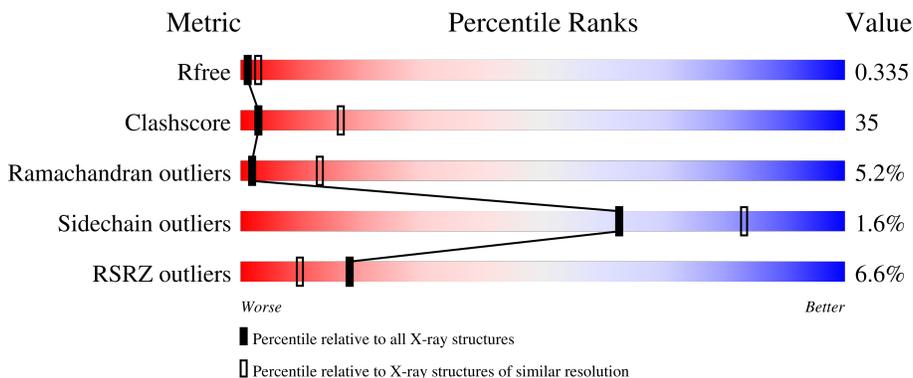
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.16 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))
$R_{free}$	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	360	 7% 26% 36% 6% 32%
1	B	360	 2% 27% 40% •• 29%
1	C	360	 6% 27% 38% • 32%
1	D	360	 3% 32% 35% • 29%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8092 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.

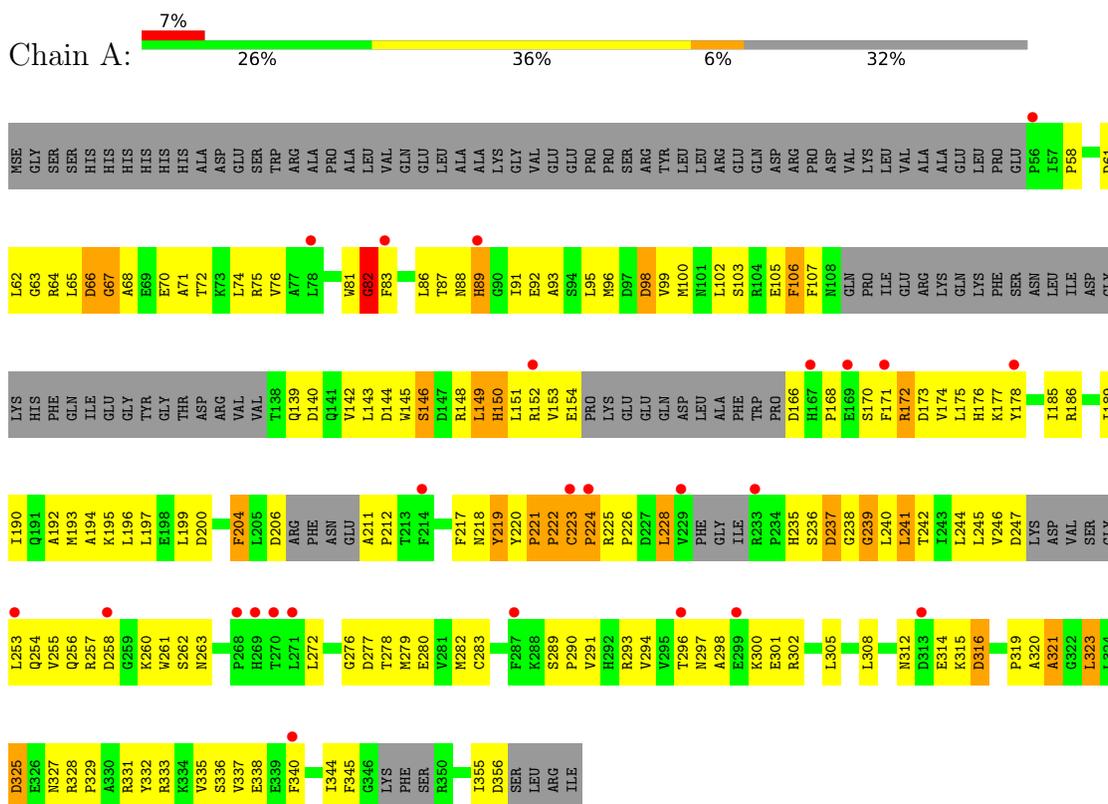
- Molecule 1 is a protein called Tri-Ketone Dioxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	246	1980	1252	349	370	3	6	0	0	0
1	D	255	2061	1313	360	379	3	6	0	0	0
1	C	246	1981	1256	349	367	3	6	0	0	0
1	B	256	2070	1318	362	381	3	6	0	0	0

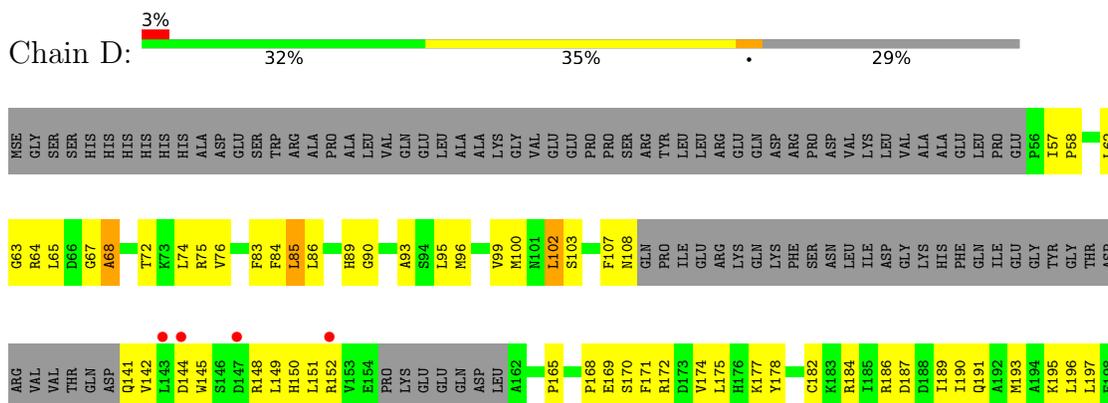
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Tri-Ketone Dioxygenase



- Molecule 1: Tri-Ketone Dioxygenase





L205	L270	K333
D206	L271	K334
ARG	L272	Y335
PHE	L273	S336
ASN	N274	Y337
GLU	L275	E338
A211	G276	F339
F212	D277	F340
T213	T278	R341
F214	N279	F345
A215	E280	G346
R216	V281	K347
F217	M282	F348
R218	G285	S349
Y219	K288	R350
Y220	S289	G351
C223	P290	E352
P224	V291	R353
R225	H292	Y354
F226	R293	I355
D227	V294	D356
L228	V295	S357
L229	T296	L358
V229	M297	ARG
F230	A298	ILE
GLY	E299	
ILE	K300	
R233	E301	
P234	R302	
H235	I303	
S236	S304	
D237	L305	
G238	A306	
G239	M307	
L240	I308	
L241	Y309	
T242		
L243		
L244		
L245		
V246		
D247		
K248		
D249		
VAL		
SER		
GLY		
L253		
Q254		
V255		
Q256		
R257		
G258		
V261		
S262		
N263		
G264		
T267		
P268		
H269		
	M312	
	D313	
	E314	
	K315	
	D316	
	I317	
	E318	
	F319	
	A320	
	A321	
	G322	
	L323	
	L324	
	D325	
	E326	
	N327	
	R328	
	F329	
	A330	
	R331	
	Y332	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.56Å 73.56Å 259.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.78 – 3.16 36.78 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.78-3.16) 99.4 (36.78-3.16)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 3.18Å)	Xtrriage
Refinement program	REFMAC 5, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.274 , 0.318 0.289 , 0.335	Depositor DCC
$R_{free}$ test set	1143 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	110.3	Xtrriage
Anisotropy	0.376	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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	0.74	1/2012 (0.0%)	1.07	4/2708 (0.1%)
1	B	0.79	2/2109 (0.1%)	1.06	8/2840 (0.3%)
1	C	0.72	1/2014 (0.0%)	1.08	9/2711 (0.3%)
1	D	0.79	2/2101 (0.1%)	1.01	7/2831 (0.2%)
All	All	0.76	6/8236 (0.1%)	1.06	28/11090 (0.3%)

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
1	B	0	3
1	C	0	1
1	D	0	1
All	All	0	6

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	261	TRP	CB-CG	-8.13	1.35	1.50
1	C	283	CYS	CB-SG	-7.18	1.70	1.82
1	D	283	CYS	CB-SG	-6.99	1.70	1.82
1	A	283	CYS	CB-SG	-6.91	1.70	1.82
1	B	81	TRP	CB-CG	-5.89	1.39	1.50

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	LEU	CA-CB-CG	7.80	133.23	115.30
1	C	245	LEU	CA-CB-CG	7.37	132.25	115.30
1	A	228	LEU	CA-CB-CG	7.33	132.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	85	LEU	CA-CB-CG	7.12	131.67	115.30
1	B	240	LEU	CA-CB-CG	7.04	131.49	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	ALA	Peptide
1	B	170	SER	Peptide
1	B	223	CYS	Peptide
1	C	355	ILE	Peptide
1	D	346	GLY	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	1980	0	1940	170	0
1	B	2070	0	2030	163	0
1	C	1981	0	1949	163	0
1	D	2061	0	2023	135	0
All	All	8092	0	7942	557	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 35.

The worst 5 of 557 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:256:GLN:CD	1:B:261:TRP:HE1	1.23	1.41
1:B:256:GLN:NE2	1:B:261:TRP:HE1	1.26	1.31
1:B:256:GLN:NE2	1:B:261:TRP:NE1	1.88	1.18
1:B:256:GLN:CD	1:B:261:TRP:NE1	2.07	1.07
1:B:253:LEU:HB3	1:B:302:ARG:HH22	1.23	1.04

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	232/360 (64%)	187 (81%)	23 (10%)	22 (10%)	0	3
1	B	244/360 (68%)	209 (86%)	27 (11%)	8 (3%)	4	22
1	C	232/360 (64%)	190 (82%)	31 (13%)	11 (5%)	2	15
1	D	245/360 (68%)	207 (84%)	29 (12%)	9 (4%)	3	19
All	All	953/1440 (66%)	793 (83%)	110 (12%)	50 (5%)	2	13

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	GLY
1	A	212	PRO
1	A	219	TYR
1	A	222	PRO
1	A	223	CYS

### 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	216/308 (70%)	210 (97%)	6 (3%)	43	73
1	B	225/308 (73%)	221 (98%)	4 (2%)	59	81
1	C	216/308 (70%)	213 (99%)	3 (1%)	67	85
1	D	224/308 (73%)	223 (100%)	1 (0%)	91	96
All	All	881/1232 (72%)	867 (98%)	14 (2%)	62	83

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	73	LYS
1	C	89	HIS
1	B	237	ASP
1	B	163	PHE
1	B	235	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	150	HIS
1	C	284	ASN
1	B	256	GLN
1	B	108	ASN
1	C	79	GLN

### 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 monosaccharides 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	240/360 (66%)	0.56	25 (10%) <b>6</b> <b>3</b>	81, 112, 152, 168	0
1	B	250/360 (69%)	0.22	7 (2%) 53 36	81, 102, 137, 156	0
1	C	240/360 (66%)	0.49	23 (9%) <b>8</b> <b>4</b>	81, 112, 153, 180	0
1	D	249/360 (69%)	0.30	10 (4%) 38 23	81, 101, 139, 159	0
All	All	979/1440 (67%)	0.39	65 (6%) <b>18</b> <b>10</b>	81, 107, 147, 180	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	224	PRO	11.8
1	C	225	ARG	8.4
1	A	171	PHE	6.7
1	C	223	CYS	6.4
1	A	287	PHE	6.3

### 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 monosaccharides 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.