



# wwPDB X-ray Structure Validation Summary Report

Sep 3, 2014 – 06:55 PM EDT

PDB ID : 4MKR  
Title : Structure of the apo form of a Zingiber officinale double bond reductase  
Authors : Buratto, J.; Langlois d'Estaintot, B.; Granier, T.; Gallois, B.; Willis, M.A.;  
Sang, Y.; Flores-Sanchez, I.J.; Gang, D.R.  
Deposited on : 2013-09-05  
Resolution : 2.58 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

---

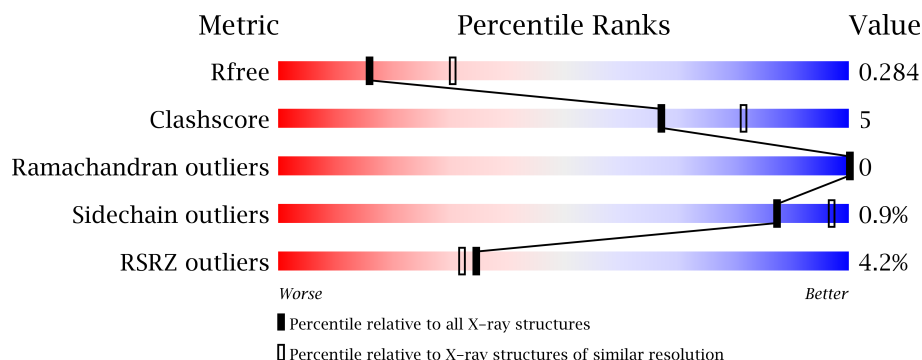
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23489
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.58 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))
$R_{free}$	66092	1891 (2.60-2.56)
Clashscore	79885	2358 (2.60-2.56)
Ramachandran outliers	78287	2316 (2.60-2.56)
Sidechain outliers	78261	2316 (2.60-2.56)
RSRZ outliers	66119	1891 (2.60-2.56)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	358	
1	B	358	
1	C	358	
1	D	358	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9244 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Zingiber officinale double bond reductase.

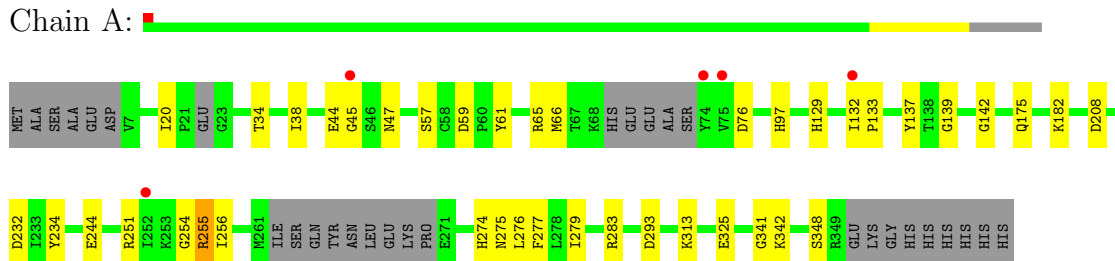
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2518	1643	406	457	12			
1	B	228	Total	C	N	O	S	0	0	0
			1644	1069	271	297	7			
1	C	330	Total	C	N	O	S	0	1	0
			2521	1644	409	456	12			
1	D	327	Total	C	N	O	S	0	0	0
			2442	1591	396	444	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	B	12	Total	O	0	0
			12	12		
2	C	43	Total	O	0	0
			43	43		
2	D	20	Total	O	0	0
			20	20		

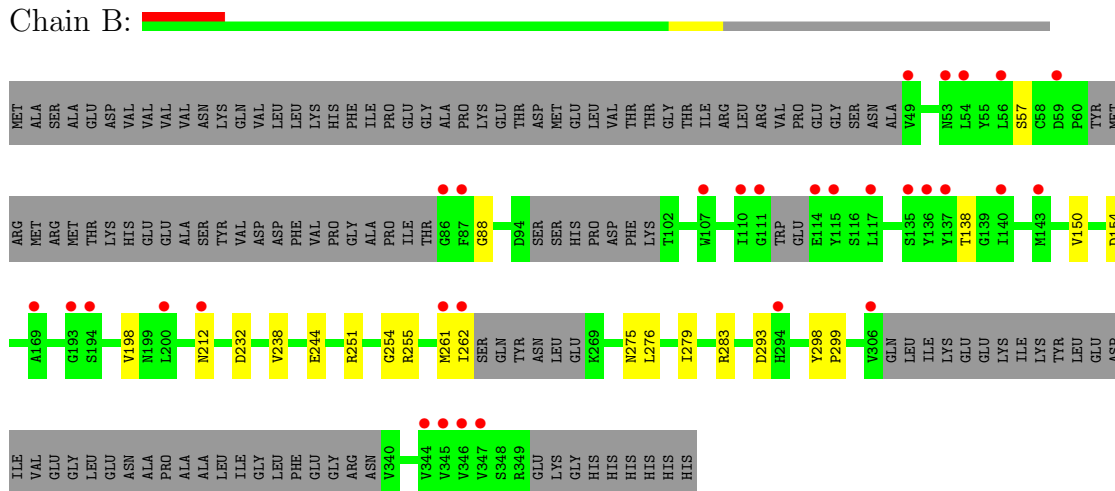
- Molecule 1: Zingiber officinale double bond reductase

Chain A:



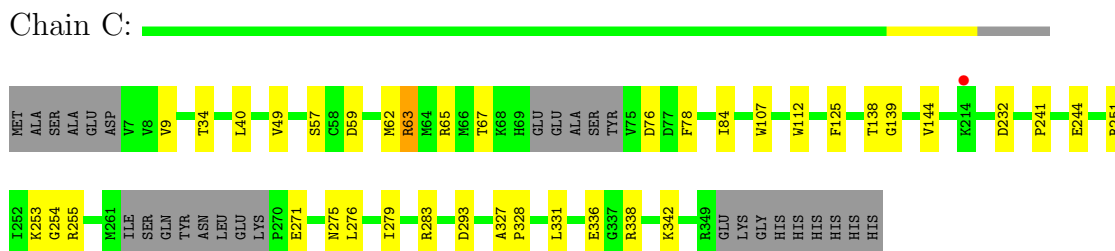
- Molecule 1: Zingiber officinale double bond reductase

Chain B:



- Molecule 1: Zingiber officinale double bond reductase

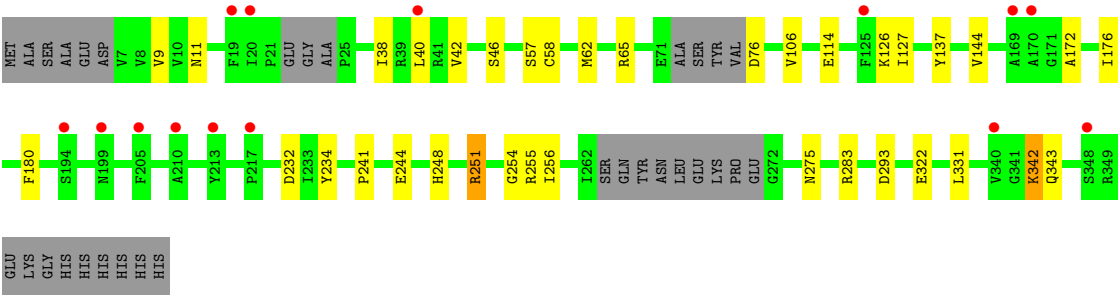
Chain C:



- Molecule 1: Zingiber officinale double bond reductase

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.93Å 76.34Å 93.45Å 80.15° 89.97° 85.66°	Depositor
Resolution (Å)	46.03 – 2.58 46.03 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.03-2.58) 97.7 (46.03-2.58)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.228 , 0.282 0.231 , 0.284	Depositor DCC
$R_{free}$ test set	2130 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42572 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	A	0.80	0/2575	0.87	3/3483 (0.1%)
1	B	0.63	0/1680	0.81	0/2278
1	C	0.78	0/2583	0.88	1/3500 (0.0%)
1	D	0.66	0/2498	0.78	1/3393 (0.0%)
All	All	0.73	0/9336	0.84	5/12654 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	GLY	N-CA-C	5.65	127.22	113.10
1	A	255	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	251	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	65	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	63	ARG	NE-CZ-NH1	-5.09	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2518	0	2491	26	0
1	B	1644	0	1480	15	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2521	0	2478	27	0
1	D	2442	0	2322	27	0
2	A	44	0	0	1	0
2	B	12	0	0	0	0
2	C	43	0	0	1	0
2	D	20	0	0	4	0
All	All	9244	0	8771	89	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 89 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:244:GLU:CB	1:A:275:ASN:HD22	2.15	0.59
1:D:65:ARG:NH1	1:D:76:ASP:O	2.35	0.59
1:A:132:ILE:HG22	1:A:133:PRO:HD2	1.84	0.58
1:D:144:VAL:HG23	2:D:407:HOH:O	2.05	0.57
1:B:254:GLY:C	1:B:255:ARG:HG3	2.25	0.56

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	A	320/358 (89%)	310 (97%)	10 (3%)	0	100	100
1	B	216/358 (60%)	206 (95%)	10 (5%)	0	100	100
1	C	325/358 (91%)	315 (97%)	10 (3%)	0	100	100
1	D	319/358 (89%)	312 (98%)	7 (2%)	0	100	100
All	All	1180/1432 (82%)	1143 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.



### 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	261/300 (87%)	257 (98%)	4 (2%)	76	93
1	B	145/300 (48%)	145 (100%)	0	100	100
1	C	259/300 (86%)	257 (99%)	2 (1%)	89	97
1	D	240/300 (80%)	238 (99%)	2 (1%)	89	97
All	All	905/1200 (75%)	897 (99%)	8 (1%)	87	97

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	SER
1	D	342	LYS
1	C	76	ASP
1	A	76	ASP
1	C	49	VAL

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	275	ASN
1	B	275	ASN
1	C	275	ASN
1	D	275	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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 ⓘ

### 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	328/358 (91%)	0.17	5 (1%) 70 71	23, 39, 58, 78	0
1	B	228/358 (63%)	0.78	31 (13%) 4 3	29, 59, 112, 152	0
1	C	330/358 (92%)	0.08	1 (0%) 91 93	22, 37, 56, 79	0
1	D	327/358 (91%)	0.34	14 (4%) 34 31	31, 52, 76, 88	0
All	All	1213/1432 (84%)	0.31	51 (4%) 35 32	22, 45, 81, 152	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	TYR	5.5
1	B	193	GLY	5.0
1	B	111	GLY	4.8
1	B	194	SER	4.6
1	B	49	VAL	3.9

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.