



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 10:25 PM GMT

PDB ID : 1MO2  
Title : Thioesterase Domain from 6-Deoxyerythronolide Synthase (DEBS TE), pH 8.5  
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Deposited on : 2002-09-05  
Resolution : 3.00 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>

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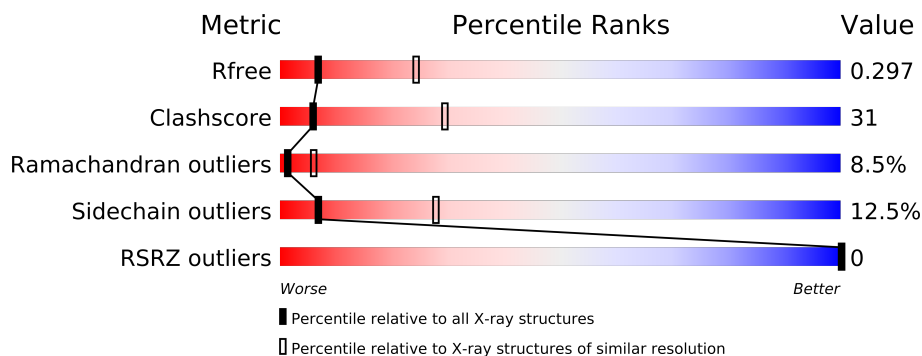
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. 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	294	
1	B	294	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3830 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 Erythronolide synthase, modules 5 and 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1887	1192	329	357	9			
1	B	251	Total	C	N	O	S	0	0	0
			1887	1192	329	357	9			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INSERTION	UNP Q03133
A	2	ALA	-	INSERTION	UNP Q03133
A	3	SER	-	INSERTION	UNP Q03133
A	284	SER	-	INSERTION	UNP Q03133
A	285	SER	-	INSERTION	UNP Q03133
A	286	VAL	-	INSERTION	UNP Q03133
A	287	ASP	-	INSERTION	UNP Q03133
A	288	LYS	-	INSERTION	UNP Q03133
A	289	LEU	-	INSERTION	UNP Q03133
A	290	ALA	-	INSERTION	UNP Q03133
A	291	ALA	-	INSERTION	UNP Q03133
A	292	ALA	-	INSERTION	UNP Q03133
A	293	LEU	-	INSERTION	UNP Q03133
A	294	GLU	-	INSERTION	UNP Q03133
B	1	MET	-	INSERTION	UNP Q03133
B	2	ALA	-	INSERTION	UNP Q03133
B	3	SER	-	INSERTION	UNP Q03133
B	284	SER	-	INSERTION	UNP Q03133
B	285	SER	-	INSERTION	UNP Q03133
B	286	VAL	-	INSERTION	UNP Q03133
B	287	ASP	-	INSERTION	UNP Q03133
B	288	LYS	-	INSERTION	UNP Q03133
B	289	LEU	-	INSERTION	UNP Q03133
B	290	ALA	-	INSERTION	UNP Q03133
B	291	ALA	-	INSERTION	UNP Q03133

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Chain	Residue	Modelled	Actual	Comment	Reference
B	292	ALA	-	INSERTION	UNP Q03133
B	293	LEU	-	INSERTION	UNP Q03133
B	294	GLU	-	INSERTION	UNP Q03133

- Molecule 2 is water.

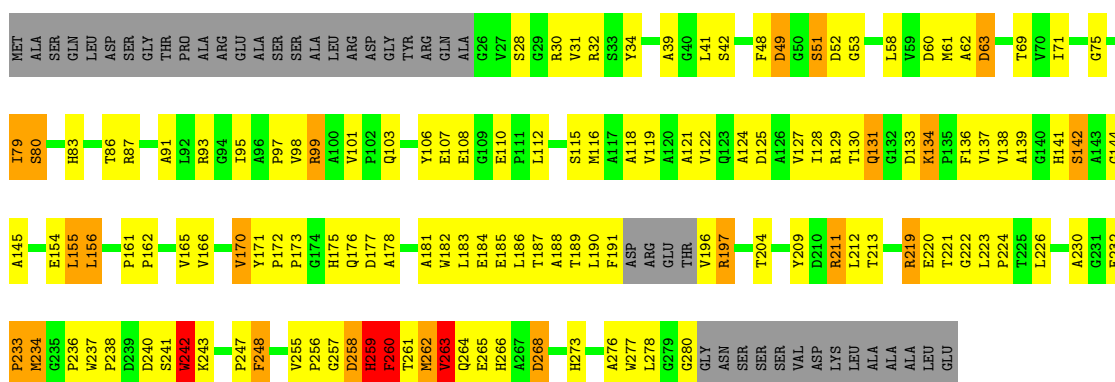
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total	O	0	0
			29	29		
2	B	27	Total	O	0	0
			27	27		

### 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 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.

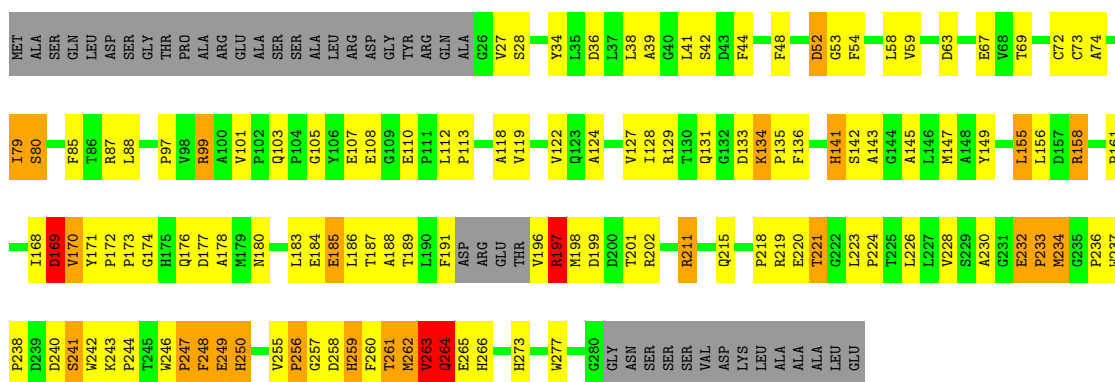
- Molecule 1: Erythronolide synthase, modules 5 and 6

Chain A:



- Molecule 1: Erythronolide synthase, modules 5 and 6

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.50Å 102.50Å 156.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 49.22 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.6 (30.00-3.00) 84.2 (49.22-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, $R_{free}$	0.242 , 0.287 0.254 , 0.297	Depositor DCC
$R_{free}$ test set	1082 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.2	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.3	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 23833 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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	0.48	0/1939	0.74	2/2651 (0.1%)
1	B	0.46	0/1939	0.73	1/2651 (0.0%)
All	All	0.47	0/3878	0.74	3/5302 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	PHE	N-CA-C	7.11	130.19	111.00
1	A	259	HIS	N-CA-C	5.28	125.24	111.00
1	B	266	HIS	N-CA-C	-5.06	97.35	111.00

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	1887	0	1810	124	1
1	B	1887	0	1810	111	1
2	A	29	0	0	3	0
2	B	27	0	0	4	0
All	All	3830	0	3620	231	1

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 31.

The worst 5 of 231 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:232:GLU:HB3	1:A:233:PRO:HD2	1.26	1.08
1:A:71:ILE:HD13	1:A:136:PHE:HB2	1.37	1.06
1:B:63:ASP:HA	1:B:97:PRO:HA	1.52	0.91
1:A:170:VAL:HG12	1:A:171:TYR:H	1.32	0.91
1:B:232:GLU:CB	1:B:233:PRO:HD2	2.00	0.91

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:261:THR:N	1:B:259:HIS:N[2.564]	2.19	0.01

## 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	247/294 (84%)	194 (78%)	32 (13%)	21 (8%)	1	6
1	B	247/294 (84%)	201 (81%)	25 (10%)	21 (8%)	1	6
All	All	494/588 (84%)	395 (80%)	57 (12%)	42 (8%)	1	6

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	233	PRO
1	A	240	ASP
1	A	256	PRO
1	A	259	HIS



### 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	192/224 (86%)	167 (87%)	25 (13%)	6	26
1	B	192/224 (86%)	169 (88%)	23 (12%)	7	30
All	All	384/448 (86%)	336 (88%)	48 (12%)	7	28

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	B	42	SER
1	B	262	MET
1	A	266	HIS
1	A	273	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	B	123	GLN
1	B	259	HIS
1	A	264	GLN
1	B	180	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	251/294 (85%)	-0.21	0 100 100	34, 52, 94, 120	0
1	B	251/294 (85%)	-0.21	0 100 100	35, 51, 91, 123	0
All	All	502/588 (85%)	-0.21	0 100 100	34, 52, 94, 123	0

There are no RSRZ outliers to report.

### 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.