



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 08:49 PM GMT

PDB ID : 2OTN  
Title : Crystal structure of the catalytically active form of diaminopimelate epimerase from *Bacillus anthracis*  
Authors : Matho, M.H.; Fukuda, K.; Santelli, E.; Jaroszewski, L.; Liddington, R.C.; Roper, D.  
Deposited on : 2007-02-08  
Resolution : 2.40 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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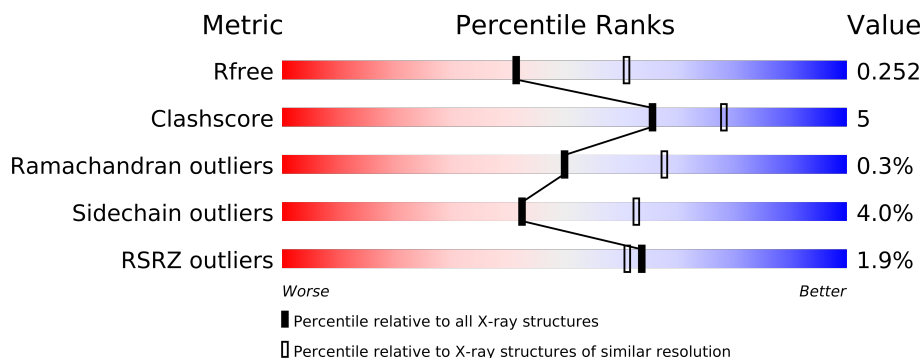
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	308	
1	B	308	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4710 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 Diaminopimelate epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2250	1419	377	434	20			
1	B	288	Total	C	N	O	S	0	0	0
			2220	1403	371	426	20			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	INITIATING METHIONINE	UNP Q81XR2
A	-18	GLY	-	EXPRESSION TAG	UNP Q81XR2
A	-17	SER	-	EXPRESSION TAG	UNP Q81XR2
A	-16	SER	-	EXPRESSION TAG	UNP Q81XR2
A	-15	HIS	-	EXPRESSION TAG	UNP Q81XR2
A	-14	HIS	-	EXPRESSION TAG	UNP Q81XR2
A	-13	HIS	-	EXPRESSION TAG	UNP Q81XR2
A	-12	HIS	-	EXPRESSION TAG	UNP Q81XR2
A	-11	HIS	-	EXPRESSION TAG	UNP Q81XR2
A	-10	HIS	-	EXPRESSION TAG	UNP Q81XR2
A	-9	SER	-	EXPRESSION TAG	UNP Q81XR2
A	-8	SER	-	EXPRESSION TAG	UNP Q81XR2
A	-7	GLY	-	EXPRESSION TAG	UNP Q81XR2
A	-6	LEU	-	EXPRESSION TAG	UNP Q81XR2
A	-5	VAL	-	EXPRESSION TAG	UNP Q81XR2
A	-4	PRO	-	EXPRESSION TAG	UNP Q81XR2
A	-3	ARG	-	EXPRESSION TAG	UNP Q81XR2
A	-2	GLY	-	EXPRESSION TAG	UNP Q81XR2
A	-1	SER	-	EXPRESSION TAG	UNP Q81XR2
A	0	HIS	-	EXPRESSION TAG	UNP Q81XR2
B	-19	MET	-	INITIATING METHIONINE	UNP Q81XR2
B	-18	GLY	-	EXPRESSION TAG	UNP Q81XR2
B	-17	SER	-	EXPRESSION TAG	UNP Q81XR2
B	-16	SER	-	EXPRESSION TAG	UNP Q81XR2
B	-15	HIS	-	EXPRESSION TAG	UNP Q81XR2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q81XR2
B	-13	HIS	-	EXPRESSION TAG	UNP Q81XR2
B	-12	HIS	-	EXPRESSION TAG	UNP Q81XR2
B	-11	HIS	-	EXPRESSION TAG	UNP Q81XR2
B	-10	HIS	-	EXPRESSION TAG	UNP Q81XR2
B	-9	SER	-	EXPRESSION TAG	UNP Q81XR2
B	-8	SER	-	EXPRESSION TAG	UNP Q81XR2
B	-7	GLY	-	EXPRESSION TAG	UNP Q81XR2
B	-6	LEU	-	EXPRESSION TAG	UNP Q81XR2
B	-5	VAL	-	EXPRESSION TAG	UNP Q81XR2
B	-4	PRO	-	EXPRESSION TAG	UNP Q81XR2
B	-3	ARG	-	EXPRESSION TAG	UNP Q81XR2
B	-2	GLY	-	EXPRESSION TAG	UNP Q81XR2
B	-1	SER	-	EXPRESSION TAG	UNP Q81XR2
B	0	HIS	-	EXPRESSION TAG	UNP Q81XR2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	125	Total O 125 125	0	0
2	B	115	Total O 115 115	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.86Å 87.33Å 110.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.23 – 2.40 36.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (36.23-2.40) 98.9 (36.22-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.180 , 0.250 0.184 , 0.252	Depositor DCC
$R_{free}$ test set	1234 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 24909 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.42 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8488e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.56	0/2292	0.68	0/3102
1	B	0.51	0/2261	0.62	0/3058
All	All	0.53	0/4553	0.65	0/6160

There are no bond length outliers.

There are no bond angle outliers.

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	2250	0	2215	22	0
1	B	2220	0	2188	24	0
2	A	125	0	0	2	0
2	B	115	0	0	6	0
All	All	4710	0	4403	46	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 46 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:131:THR:HG21	2:B:393:HOH:O	1.76	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:275:GLU:OE2	2:B:392:HOH:O	2.03	0.76
1:A:42:ASN:HB3	2:B:396:HOH:O	1.88	0.74
1:A:193:MET:HE3	2:A:339:HOH:O	1.91	0.68
1:B:166:ASN:HD22	1:B:166:ASN:H	1.42	0.68

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	291/308 (94%)	282 (97%)	8 (3%)	1 (0%)	50	68
1	B	284/308 (92%)	272 (96%)	11 (4%)	1 (0%)	43	61
All	All	575/616 (93%)	554 (96%)	19 (3%)	2 (0%)	50	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	CYS
1	A	76	CYS

### 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	242/254 (95%)	234 (97%)	8 (3%)	50	71
1	B	239/254 (94%)	228 (95%)	11 (5%)	37	55
All	All	481/508 (95%)	462 (96%)	19 (4%)	42	63



5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	20	ASN
1	B	58	VAL
1	B	192	GLU
1	A	279	ARG
1	B	193	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	HIS
1	B	252	HIS
1	B	166	ASN
1	A	166	ASN
1	B	20	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	293/308 (95%)	-0.26	0 <span>100</span> <span>100</span>	11, 29, 48, 69	0
1	B	288/308 (93%)	0.06	11 (3%) <span>38</span> <span>36</span>	3, 30, 48, 62	0
All	All	581/616 (94%)	-0.10	11 (1%) <span>64</span> <span>61</span>	3, 30, 48, 69	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	GLN	4.5
1	B	183	THR	4.3
1	B	182	THR	4.2
1	B	94	GLU	3.9
1	B	226	CYS	3.8

### 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.