



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:19 PM GMT

PDB ID : 4EGJ  
Title : Crystal structure of D-alanine-D-alanine ligase from Burkholderia xenovorans  
Authors : Ssgcid; Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2012-03-31  
Resolution : 2.30 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  
<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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

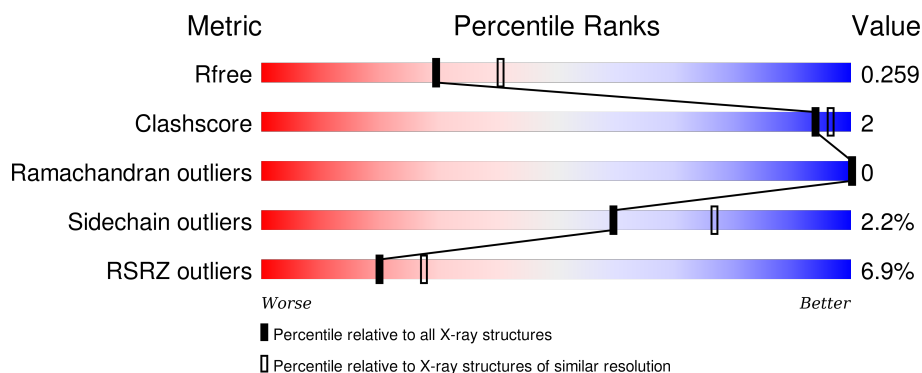
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	334	<div> <div>3%</div> <div>81%</div> <div>15%</div> </div>
1	B	334	<div> <div>3%</div> <div>78%</div> <div>7%</div> <div>15%</div> </div>
1	C	334	<div> <div>13%</div> <div>81%</div> <div>15%</div> </div>
1	D	334	<div> <div>4%</div> <div>70%</div> <div>26%</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8430 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 D-alanine–D-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	3	0
			2118	1357	365	390	6			
1	B	285	Total	C	N	O	S	0	2	0
			2099	1344	362	387	6			
1	C	283	Total	C	N	O	S	0	0	0
			2033	1291	352	385	5			
1	D	246	Total	C	N	O	S	0	0	0
			1822	1162	314	341	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	INITIATING METHIONINE	UNP Q13TZ4
A	-19	ALA	-	EXPRESSION TAG	UNP Q13TZ4
A	-18	HIS	-	EXPRESSION TAG	UNP Q13TZ4
A	-17	HIS	-	EXPRESSION TAG	UNP Q13TZ4
A	-16	HIS	-	EXPRESSION TAG	UNP Q13TZ4
A	-15	HIS	-	EXPRESSION TAG	UNP Q13TZ4
A	-14	HIS	-	EXPRESSION TAG	UNP Q13TZ4
A	-13	HIS	-	EXPRESSION TAG	UNP Q13TZ4
A	-12	MET	-	EXPRESSION TAG	UNP Q13TZ4
A	-11	GLY	-	EXPRESSION TAG	UNP Q13TZ4
A	-10	THR	-	EXPRESSION TAG	UNP Q13TZ4
A	-9	LEU	-	EXPRESSION TAG	UNP Q13TZ4
A	-8	GLU	-	EXPRESSION TAG	UNP Q13TZ4
A	-7	ALA	-	EXPRESSION TAG	UNP Q13TZ4
A	-6	GLN	-	EXPRESSION TAG	UNP Q13TZ4
A	-5	THR	-	EXPRESSION TAG	UNP Q13TZ4
A	-4	GLN	-	EXPRESSION TAG	UNP Q13TZ4
A	-3	GLY	-	EXPRESSION TAG	UNP Q13TZ4
A	-2	PRO	-	EXPRESSION TAG	UNP Q13TZ4
A	-1	GLY	-	EXPRESSION TAG	UNP Q13TZ4
A	0	SER	-	EXPRESSION TAG	UNP Q13TZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	INITIATING METHIONINE	UNP Q13TZ4
B	-19	ALA	-	EXPRESSION TAG	UNP Q13TZ4
B	-18	HIS	-	EXPRESSION TAG	UNP Q13TZ4
B	-17	HIS	-	EXPRESSION TAG	UNP Q13TZ4
B	-16	HIS	-	EXPRESSION TAG	UNP Q13TZ4
B	-15	HIS	-	EXPRESSION TAG	UNP Q13TZ4
B	-14	HIS	-	EXPRESSION TAG	UNP Q13TZ4
B	-13	HIS	-	EXPRESSION TAG	UNP Q13TZ4
B	-12	MET	-	EXPRESSION TAG	UNP Q13TZ4
B	-11	GLY	-	EXPRESSION TAG	UNP Q13TZ4
B	-10	THR	-	EXPRESSION TAG	UNP Q13TZ4
B	-9	LEU	-	EXPRESSION TAG	UNP Q13TZ4
B	-8	GLU	-	EXPRESSION TAG	UNP Q13TZ4
B	-7	ALA	-	EXPRESSION TAG	UNP Q13TZ4
B	-6	GLN	-	EXPRESSION TAG	UNP Q13TZ4
B	-5	THR	-	EXPRESSION TAG	UNP Q13TZ4
B	-4	GLN	-	EXPRESSION TAG	UNP Q13TZ4
B	-3	GLY	-	EXPRESSION TAG	UNP Q13TZ4
B	-2	PRO	-	EXPRESSION TAG	UNP Q13TZ4
B	-1	GLY	-	EXPRESSION TAG	UNP Q13TZ4
B	0	SER	-	EXPRESSION TAG	UNP Q13TZ4
C	-20	MET	-	INITIATING METHIONINE	UNP Q13TZ4
C	-19	ALA	-	EXPRESSION TAG	UNP Q13TZ4
C	-18	HIS	-	EXPRESSION TAG	UNP Q13TZ4
C	-17	HIS	-	EXPRESSION TAG	UNP Q13TZ4
C	-16	HIS	-	EXPRESSION TAG	UNP Q13TZ4
C	-15	HIS	-	EXPRESSION TAG	UNP Q13TZ4
C	-14	HIS	-	EXPRESSION TAG	UNP Q13TZ4
C	-13	HIS	-	EXPRESSION TAG	UNP Q13TZ4
C	-12	MET	-	EXPRESSION TAG	UNP Q13TZ4
C	-11	GLY	-	EXPRESSION TAG	UNP Q13TZ4
C	-10	THR	-	EXPRESSION TAG	UNP Q13TZ4
C	-9	LEU	-	EXPRESSION TAG	UNP Q13TZ4
C	-8	GLU	-	EXPRESSION TAG	UNP Q13TZ4
C	-7	ALA	-	EXPRESSION TAG	UNP Q13TZ4
C	-6	GLN	-	EXPRESSION TAG	UNP Q13TZ4
C	-5	THR	-	EXPRESSION TAG	UNP Q13TZ4
C	-4	GLN	-	EXPRESSION TAG	UNP Q13TZ4
C	-3	GLY	-	EXPRESSION TAG	UNP Q13TZ4
C	-2	PRO	-	EXPRESSION TAG	UNP Q13TZ4
C	-1	GLY	-	EXPRESSION TAG	UNP Q13TZ4
C	0	SER	-	EXPRESSION TAG	UNP Q13TZ4

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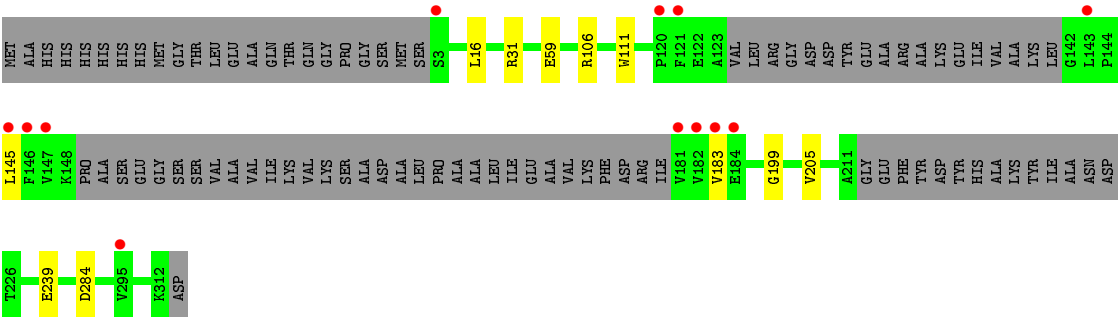
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	INITIATING METHIONINE	UNP Q13TZ4
D	-19	ALA	-	EXPRESSION TAG	UNP Q13TZ4
D	-18	HIS	-	EXPRESSION TAG	UNP Q13TZ4
D	-17	HIS	-	EXPRESSION TAG	UNP Q13TZ4
D	-16	HIS	-	EXPRESSION TAG	UNP Q13TZ4
D	-15	HIS	-	EXPRESSION TAG	UNP Q13TZ4
D	-14	HIS	-	EXPRESSION TAG	UNP Q13TZ4
D	-13	HIS	-	EXPRESSION TAG	UNP Q13TZ4
D	-12	MET	-	EXPRESSION TAG	UNP Q13TZ4
D	-11	GLY	-	EXPRESSION TAG	UNP Q13TZ4
D	-10	THR	-	EXPRESSION TAG	UNP Q13TZ4
D	-9	LEU	-	EXPRESSION TAG	UNP Q13TZ4
D	-8	GLU	-	EXPRESSION TAG	UNP Q13TZ4
D	-7	ALA	-	EXPRESSION TAG	UNP Q13TZ4
D	-6	GLN	-	EXPRESSION TAG	UNP Q13TZ4
D	-5	THR	-	EXPRESSION TAG	UNP Q13TZ4
D	-4	GLN	-	EXPRESSION TAG	UNP Q13TZ4
D	-3	GLY	-	EXPRESSION TAG	UNP Q13TZ4
D	-2	PRO	-	EXPRESSION TAG	UNP Q13TZ4
D	-1	GLY	-	EXPRESSION TAG	UNP Q13TZ4
D	0	SER	-	EXPRESSION TAG	UNP Q13TZ4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	113	Total	O	0	0
			113	113		
2	B	98	Total	O	0	0
			98	98		
2	C	69	Total	O	0	0
			69	69		
2	D	78	Total	O	0	0
			78	78		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.93Å 78.93Å 224.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 2.30 44.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.99-2.30) 97.8 (44.76-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.224 , 0.260 0.222 , 0.259	Depositor DCC
$R_{free}$ test set	3073 reflections (5.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.9	EDS
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 59384 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8430	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 61.77 % 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 1.2460e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 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	0.77	1/2167 (0.0%)	0.86	1/2948 (0.0%)
1	B	0.78	0/2144	0.87	3/2917 (0.1%)
1	C	0.78	0/2071	0.90	5/2820 (0.2%)
1	D	0.84	1/1858 (0.1%)	0.90	2/2525 (0.1%)
All	All	0.79	2/8240 (0.0%)	0.88	11/11210 (0.1%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	TRP	CD2-CE2	5.17	1.47	1.41
1	D	111	TRP	CD2-CE2	5.14	1.47	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	31	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	C	31	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	D	106	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	301	GLU	OE1-CD-OE2	-6.22	115.84	123.30
1	C	229	LEU	CB-CG-CD2	-5.90	100.97	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	256	THR	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	2118	0	2109	8	0
1	B	2099	0	2079	13	0
1	C	2033	0	1925	3	0
1	D	1822	0	1781	4	0
2	A	113	0	0	2	0
2	B	98	0	0	1	0
2	C	69	0	0	0	0
2	D	78	0	0	1	0
All	All	8430	0	7894	28	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 2.

The worst 5 of 28 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:175:VAL:O	1:A:175:VAL:HG12	1.93	0.69
1:D:145:LEU:HD13	1:D:183:VAL:CG1	2.23	0.68
1:A:175:VAL:O	1:A:175:VAL:CG1	2.47	0.63
1:B:143:LEU:HD13	1:B:162:LYS:O	1.99	0.62
1:B:228:TYR:O	1:B:290:LYS:NZ	2.37	0.58

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	282/334 (84%)	277 (98%)	5 (2%)	0	100	100
1	B	281/334 (84%)	276 (98%)	5 (2%)	0	100	100
1	C	275/334 (82%)	268 (98%)	7 (2%)	0	100	100
1	D	238/334 (71%)	234 (98%)	4 (2%)	0	100	100
All	All	1076/1336 (80%)	1055 (98%)	21 (2%)	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	210/258 (81%)	205 (98%)	5 (2%)	57	74
1	B	206/258 (80%)	201 (98%)	5 (2%)	57	74
1	C	189/258 (73%)	185 (98%)	4 (2%)	61	78
1	D	181/258 (70%)	178 (98%)	3 (2%)	68	83
All	All	786/1032 (76%)	769 (98%)	17 (2%)	60	77

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	LEU
1	B	172	ILE
1	C	284	ASP
1	B	16	LEU
1	D	16	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

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	285/334 (85%)	0.21	10 (3%) 48 56	19, 27, 55, 72	0
1	B	285/334 (85%)	0.19	9 (3%) 51 60	18, 26, 63, 82	0
1	C	283/334 (84%)	0.91	45 (15%) 3 4	21, 31, 91, 112	0
1	D	246/334 (73%)	0.13	12 (4%) 33 42	18, 25, 61, 82	0
All	All	1099/1336 (82%)	0.37	76 (6%) 20 27	18, 27, 69, 112	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	ALA	13.8
1	C	166	ALA	10.4
1	C	177	PHE	10.1
1	C	172	ILE	10.0
1	C	174	ALA	9.0

### 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.