



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:22 PM GMT

PDB ID : 3TQT  
Title : Structure of the D-alanine-D-alanine ligase from *Coxiella burnetii*  
Authors : Rudolph, M.; Cheung, J.; Franklin, M.C.; Cassidy, M.; Gary, E.; Burshteyn, F.; Love, J.  
Deposited on : 2011-09-09  
Resolution : 1.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

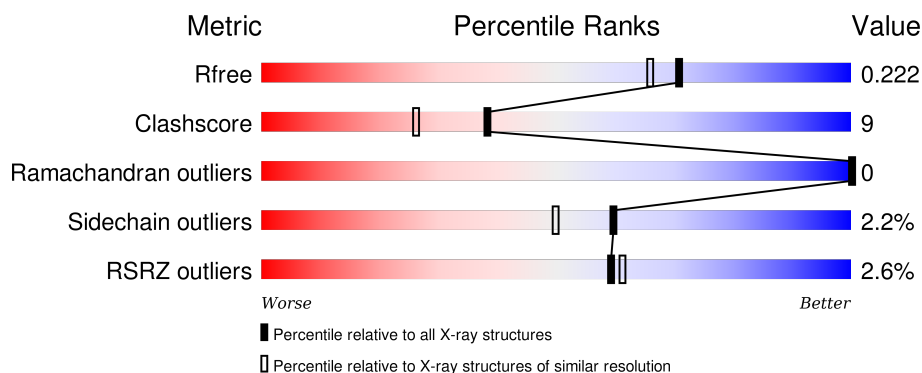
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


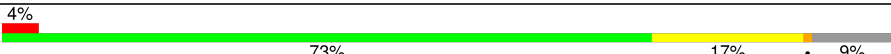
The reported resolution of this entry is 1.88 Å.

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	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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	372	 75% 18% • 6%
1	B	372	 4% 73% 17% • 9%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5830 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.

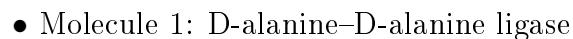
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2710	1720	468	507	15			
1	B	337	Total	C	N	O	S	0	0	0
			2630	1671	452	492	15			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	259	Total	O	0	0
			259	259		
2	B	231	Total	O	0	0
			231	231		



- Molecule 1: D-alanine–D-alanine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.24Å 97.44Å 106.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.65 – 1.88 39.65 – 1.88	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.65-1.88) 96.8 (39.65-1.88)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 1.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.180 , 0.224 0.177 , 0.222	Depositor DCC
$R_{free}$ test set	2873 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 56801 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.36	0/2763	0.53	0/3748
1	B	0.35	0/2680	0.53	0/3632
All	All	0.36	0/5443	0.53	0/7380

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2710	0	2726	58	0
1	B	2630	0	2648	52	0
2	A	259	0	0	8	0
2	B	231	0	0	7	0
All	All	5830	0	5374	97	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 9.

All (97) 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:149:ARG:HG3	1:A:149:ARG:HH11	1.05	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLN:HE21	1:B:140:GLU:HG3	1.10	1.09
1:A:133:GLN:NE2	1:B:140:GLU:HG3	1.85	0.91
1:A:149:ARG:HG3	1:A:149:ARG:NH1	1.85	0.83
1:A:149:ARG:CG	1:A:149:ARG:HH11	1.89	0.82
1:A:230:ILE:HG21	1:A:283:ILE:HD13	1.63	0.80
1:A:109:THR:HG22	1:A:110:GLN:HG2	1.71	0.73
1:B:299:MET:HE3	1:B:329:TYR:CE2	2.27	0.70
1:B:169:GLY:O	1:B:173:ARG:HG3	1.93	0.68
1:A:133:GLN:HE21	1:B:140:GLU:CG	2.00	0.68
1:A:33:ASP:HB3	1:A:36:LYS:HG3	1.75	0.68
1:B:339:PRO:HB2	1:B:342:ASN:HD22	1.59	0.66
1:A:133:GLN:NE2	1:B:140:GLU:CG	2.59	0.65
1:B:109:THR:HG22	1:B:110:GLN:HG3	1.77	0.65
1:A:112:GLU:HG2	1:A:320:ILE:CG1	2.29	0.62
1:A:215:TYR:OH	1:B:368:LYS:HG3	1.99	0.62
1:B:112:GLU:HG2	1:B:320:ILE:CG1	2.30	0.61
1:B:4:LYS:N	2:B:593:HOH:O	2.33	0.61
1:A:110:GLN:HG3	2:A:582:HOH:O	1.99	0.61
1:B:62:HIS:HD2	2:B:497:HOH:O	1.84	0.60
1:A:197:LEU:HD11	1:A:211:GLU:HG2	1.83	0.60
1:A:355:HIS:O	1:A:359:GLN:HG2	2.02	0.59
1:A:299:MET:HE3	1:A:329:TYR:CE2	2.38	0.59
1:B:339:PRO:HB2	1:B:342:ASN:ND2	2.17	0.59
1:A:13:GLY:O	1:A:18:HIS:HD2	1.84	0.59
1:B:85:LYS:N	2:B:396:HOH:O	2.36	0.58
1:A:192:SER:HB3	1:B:365:TYR:OH	2.03	0.58
1:B:228:ARG:HD2	1:B:247:GLU:OE2	2.04	0.57
1:A:186:LYS:HG2	1:A:196:THR:HG23	1.86	0.57
1:B:151:GLY:HA3	1:B:293:MET:SD	2.45	0.56
1:A:136:ALA:HB1	1:B:133:GLN:HG3	1.88	0.56
1:A:241:LYS:HE2	2:A:605:HOH:O	2.05	0.56
1:B:85:LYS:HE2	1:B:98:SER:OG	2.06	0.56
1:A:228:ARG:HD2	1:A:247:GLU:OE2	2.05	0.55
1:B:299:MET:HE3	1:B:329:TYR:CZ	2.40	0.55
1:B:10:LEU:HD13	1:B:102:VAL:HG13	1.89	0.55
1:A:354:ARG:NH1	2:A:627:HOH:O	2.38	0.55
1:A:119:LEU:HD13	1:B:119:LEU:HD13	1.88	0.55
1:B:345:ASP:O	1:B:349:GLU:HG3	2.07	0.55
1:B:359:GLN:O	1:B:363:ARG:HD3	2.07	0.55
1:A:248:ILE:HG13	1:A:269:THR:HG22	1.88	0.54
1:B:13:GLY:O	1:B:18:HIS:HD2	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLU:CG	1:B:320:ILE:HB	2.38	0.53
1:B:77:THR:HG22	1:B:90:LEU:HD21	1.91	0.53
1:B:311:LYS:HE2	1:B:313:LEU:HD21	1.91	0.52
1:A:238:GLY:O	1:A:240:PRO:HD3	2.10	0.52
1:B:112:GLU:HG2	1:B:320:ILE:HG12	1.90	0.52
1:B:219:LEU:C	1:B:219:LEU:HD12	2.30	0.52
1:B:139:MET:HE1	2:B:600:HOH:O	2.09	0.51
1:B:362:ILE:O	1:B:366:GLU:HG3	2.11	0.50
1:B:197:LEU:HD11	1:B:211:GLU:HG2	1.94	0.50
1:B:20:ILE:HG13	2:B:568:HOH:O	2.11	0.50
1:A:112:GLU:HG2	1:A:320:ILE:HG12	1.93	0.50
1:A:78:ILE:CD1	1:A:119:LEU:HD11	2.42	0.49
1:A:194:VAL:HG11	1:B:368:LYS:HB3	1.95	0.48
1:A:299:MET:HE3	1:A:329:TYR:CZ	2.49	0.48
1:A:273:VAL:HG23	1:A:275:LEU:HG	1.94	0.48
1:A:112:GLU:O	1:A:135:SER:HB3	2.14	0.47
1:A:339:PRO:HB2	1:A:342:ASN:HD22	1.78	0.47
1:B:327:SER:O	1:B:331:LYS:HG2	2.14	0.47
1:B:309:ASN:O	1:B:310:ASN:HB2	2.16	0.46
1:A:363:ARG:HH12	1:A:370:ARG:NH2	2.13	0.46
1:A:2:ALA:N	2:A:631:HOH:O	2.47	0.46
1:A:330:PRO:O	1:A:334:GLU:HG3	2.15	0.46
1:A:151:GLY:HA3	1:A:293:MET:SD	2.56	0.46
1:B:93:ASP:N	2:B:404:HOH:O	2.48	0.45
1:A:36:LYS:HD3	2:A:549:HOH:O	2.16	0.45
1:B:77:THR:CG2	1:B:90:LEU:HD21	2.47	0.45
1:B:362:ILE:HA	1:B:362:ILE:HD12	1.83	0.45
1:A:182:GLU:HB3	1:A:224:ARG:HE	1.81	0.44
1:B:67:LEU:HD22	1:B:72:SER:OG	2.17	0.44
1:A:16:THR:HG23	1:A:17:GLU:OE2	2.18	0.44
1:A:164:ARG:CZ	1:B:238:GLY:HA3	2.48	0.44
1:A:78:ILE:O	1:B:77:THR:OG1	2.31	0.44
1:B:18:HIS:CE1	1:B:22:ILE:HD11	2.53	0.44
1:A:249:ILE:HA	1:A:250:PRO:HD2	1.85	0.44
1:B:241:LYS:HE2	2:B:574:HOH:O	2.18	0.44
1:A:219:LEU:C	1:A:219:LEU:HD12	2.39	0.44
1:A:275:LEU:HD13	1:A:283:ILE:HD12	2.00	0.43
1:A:109:THR:HG21	2:A:463:HOH:O	2.17	0.43
1:A:299:MET:HB3	1:A:347:LEU:HD21	2.00	0.43
1:B:331:LYS:HD2	1:B:331:LYS:HA	1.75	0.43
1:A:112:GLU:HG2	1:A:320:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:NH1	2:A:558:HOH:O	2.50	0.43
1:A:74:ARG:HD3	1:A:97:TYR:OH	2.19	0.42
1:A:112:GLU:CG	1:A:320:ILE:HB	2.50	0.42
1:B:186:LYS:HG2	1:B:196:THR:HG23	2.00	0.42
1:B:248:ILE:HD11	1:B:328:MET:HG3	2.02	0.42
1:A:277:GLU:O	1:A:281:LYS:HG2	2.20	0.42
1:A:149:ARG:CG	1:A:149:ARG:NH1	2.59	0.41
1:B:363:ARG:O	1:B:367:VAL:HG23	2.19	0.41
1:B:126:PRO:HG3	1:B:355:HIS:CG	2.55	0.41
1:A:10:LEU:HD12	1:A:42:ILE:HB	2.03	0.41
1:A:112:GLU:HG2	1:A:320:ILE:CB	2.51	0.40
1:A:226:ARG:NH1	2:A:409:HOH:O	2.54	0.40
1:A:368:LYS:HG2	1:B:215:TYR:OH	2.22	0.40
1:A:48:GLY:O	1:B:80:PHE:HB3	2.21	0.40

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	340/372 (91%)	331 (97%)	9 (3%)	0	100	100
1	B	327/372 (88%)	324 (99%)	3 (1%)	0	100	100
All	All	667/744 (90%)	655 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	299/318 (94%)	292 (98%)	7 (2%)	58	48
1	B	292/318 (92%)	286 (98%)	6 (2%)	61	52
All	All	591/636 (93%)	578 (98%)	13 (2%)	60	50

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ARG
1	A	103	PHE
1	A	149	ARG
1	A	183	LEU
1	A	200	LYS
1	A	277	GLU
1	A	323	PHE
1	B	103	PHE
1	B	183	LEU
1	B	281	LYS
1	B	309	ASN
1	B	323	PHE
1	B	363	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	18	HIS
1	A	46	HIS
1	A	133	GLN
1	A	342	ASN
1	A	355	HIS
1	A	356	GLN
1	B	18	HIS
1	B	62	HIS
1	B	124	ASN
1	B	295	HIS
1	B	342	ASN
1	B	355	HIS
1	B	359	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 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 ⓘ

### 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	348/372 (93%)	-0.02	4 (1%) 82 84	17, 29, 49, 77	0
1	B	337/372 (90%)	0.14	14 (4%) 40 42	19, 31, 54, 75	0
All	All	685/744 (92%)	0.06	18 (2%) 59 61	17, 30, 52, 77	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	ILE	3.3
1	B	277	GLU	3.2
1	B	224	ARG	3.2
1	B	181	SER	2.8
1	B	225	ILE	2.8
1	A	132	VAL	2.8
1	B	363	ARG	2.6
1	B	138	CYS	2.6
1	B	366	GLU	2.4
1	B	176	ASP	2.4
1	B	132	VAL	2.3
1	B	268	THR	2.2
1	B	175	LEU	2.2
1	B	269	THR	2.1
1	A	277	GLU	2.1
1	B	309	ASN	2.1
1	A	194	VAL	2.1
1	A	130	ALA	2.0

### 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 [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.