



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:41 PM GMT

PDB ID : 4WD3  
Title : Crystal structure of an L-amino acid ligase RizA  
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Deposited on : 2014-09-06  
Resolution : 2.80 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

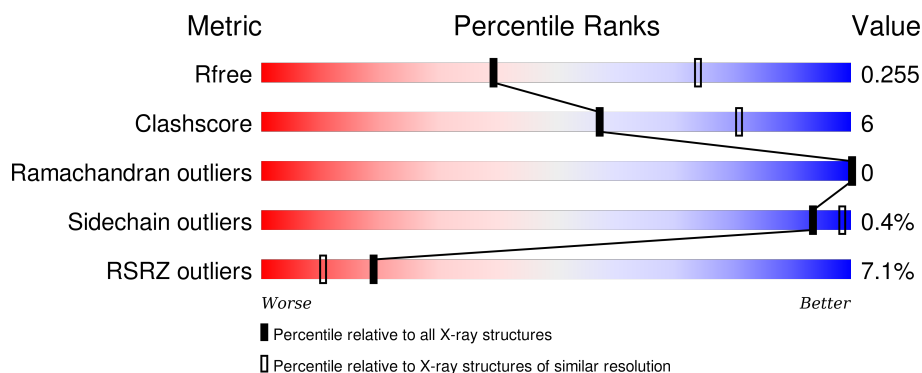
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	413	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>6%</div> </div> </div>
1	B	413	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6114 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 L-amino acid ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	Se	0	0	0
			3057	1970	489	582	6	10			
1	B	388	Total	C	N	O	S	Se	0	0	0
			3057	1970	489	582	6	10			

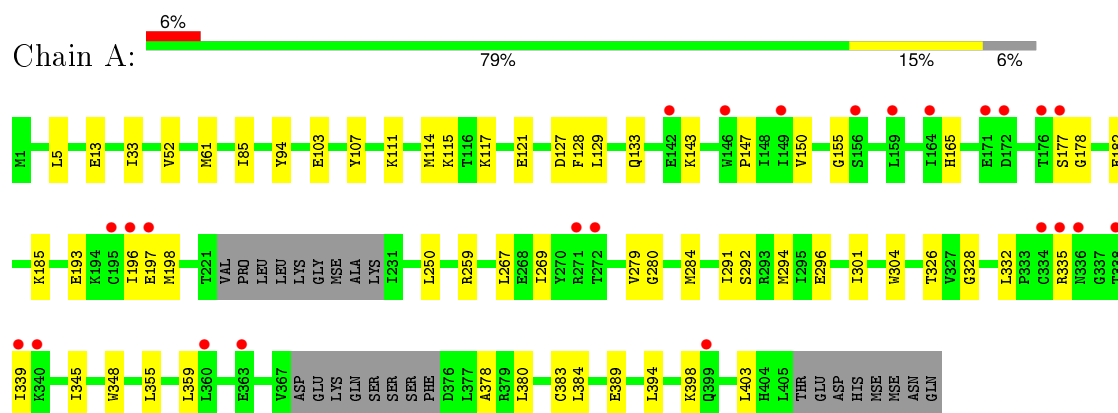
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP B5UAT8
A	74	ILE	PHE	engineered mutation	UNP B5UAT8
B	2	VAL	LEU	engineered mutation	UNP B5UAT8
B	74	ILE	PHE	engineered mutation	UNP B5UAT8

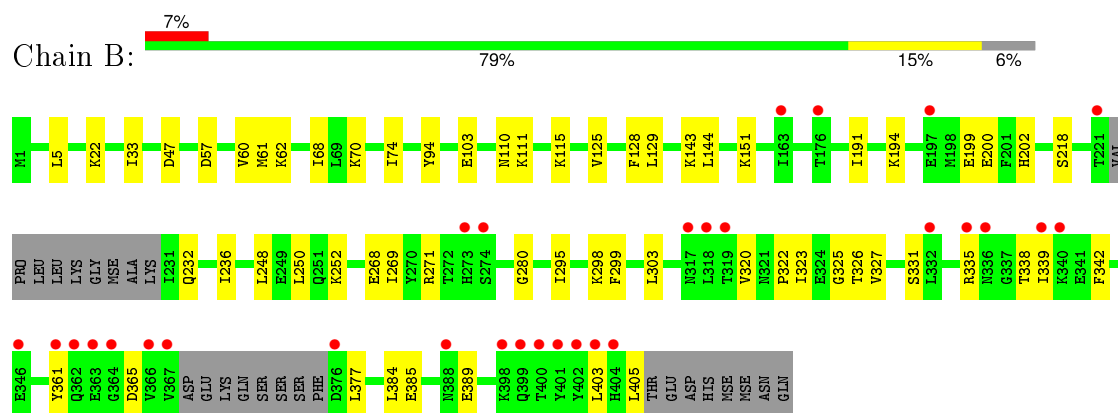
### 3 Residue-property plots [i](#)

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: L-amino acid ligase



- Molecule 1: L-amino acid ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.38Å 87.29Å 85.26Å 90.00° 97.52° 90.00°	Depositor
Resolution (Å)	48.24 – 2.80 48.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.24-2.80) 97.4 (48.24-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.71 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.201 , 0.255 0.202 , 0.255	Depositor DCC
$R_{free}$ test set	1055 reflections (5.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 20504 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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	0.22	0/3110	0.40	0/4198
1	B	0.22	0/3110	0.41	0/4198
All	All	0.22	0/6220	0.41	0/8396

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	3057	0	3065	38	0
1	B	3057	0	3065	39	0
All	All	6114	0	6130	74	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 6.

All (74) 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:115:LYS:NZ	1:A:280:GLY:O	2.12	0.82
1:B:129:LEU:HD11	1:B:143:LYS:HD3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LYS:HG3	1:B:125:VAL:HG11	1.71	0.71
1:A:111:LYS:NZ	1:A:155:GLY:O	2.24	0.70
1:A:117:LYS:NZ	1:A:121:GLU:OE2	2.31	0.64
1:A:52:VAL:HG21	1:A:61:MSE:HE1	1.80	0.63
1:B:335:ARG:NH2	1:B:403:LEU:O	2.32	0.63
1:A:103:GLU:OE1	1:A:259:ARG:NH2	2.33	0.62
1:A:127:ASP:O	1:A:193:GLU:HG3	2.01	0.60
1:A:94:TYR:O	1:B:110:ASN:ND2	2.36	0.58
1:A:326:THR:N	1:A:384:LEU:O	2.38	0.54
1:A:250:LEU:HD23	1:A:269:ILE:HD12	1.89	0.54
1:B:111:LYS:NZ	1:B:151:LYS:HD2	2.22	0.54
1:B:384:LEU:HD13	1:B:389:GLU:HB3	1.90	0.53
1:A:339:ILE:HD12	1:A:403:LEU:HD11	1.90	0.53
1:B:326:THR:N	1:B:384:LEU:O	2.32	0.53
1:B:338:THR:OG1	1:B:338:THR:O	2.25	0.53
1:A:103:GLU:HG3	1:B:103:GLU:HG3	1.92	0.51
1:B:250:LEU:HD23	1:B:269:ILE:HD12	1.92	0.51
1:A:384:LEU:HD13	1:A:389:GLU:HB3	1.93	0.50
1:B:199:GLU:OE1	1:B:271:ARG:NH2	2.44	0.50
1:A:5:LEU:HD11	1:A:33:ILE:HG13	1.94	0.49
1:B:115:LYS:NZ	1:B:280:GLY:O	2.46	0.49
1:B:232:GLN:HB2	1:B:331:SER:OG	2.13	0.49
1:A:114:MSE:SE	1:A:115:LYS:HZ2	2.46	0.48
1:B:22:LYS:NZ	1:B:47:ASP:OD2	2.32	0.48
1:A:61:MSE:HE2	1:A:61:MSE:HA	1.95	0.48
1:A:115:LYS:HB3	1:A:128:PHE:CE1	2.48	0.48
1:B:320:VAL:HG12	1:B:322:PRO:HG3	1.95	0.47
1:A:182:GLU:HA	1:A:185:LYS:HD3	1.96	0.47
1:A:85:ILE:HD12	1:A:284:MSE:HE2	1.96	0.47
1:B:202:HIS:CE1	1:B:218:SER:HB2	2.48	0.47
1:A:345:ILE:HD11	1:A:359:LEU:HD11	1.95	0.47
1:A:335:ARG:NH2	1:A:403:LEU:O	2.47	0.47
1:A:185:LYS:N	1:A:185:LYS:HD2	2.30	0.47
1:B:295:ILE:HD12	1:B:303:LEU:HD11	1.97	0.47
1:A:129:LEU:HD11	1:A:143:LYS:HD3	1.97	0.46
1:A:394:LEU:O	1:A:398:LYS:HB2	2.16	0.46
1:B:248:LEU:O	1:B:252:LYS:HG2	2.16	0.46
1:A:185:LYS:HD2	1:A:185:LYS:H	1.81	0.45
1:A:177:SER:HA	1:A:178:GLY:HA2	1.59	0.45
1:A:355:LEU:HD11	1:A:383:CYS:HB2	1.99	0.45
1:B:361:TYR:HD2	1:B:377:LEU:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:MSE:SE	1:A:328:GLY:HA2	2.67	0.45
1:B:385:GLU:N	1:B:389:GLU:OE1	2.48	0.45
1:A:267:LEU:HD11	1:A:279:VAL:HG13	1.98	0.45
1:A:107:TYR:CZ	1:A:117:LYS:HG3	2.52	0.45
1:B:5:LEU:HD11	1:B:33:ILE:HG13	1.99	0.44
1:B:129:LEU:HG	1:B:144:LEU:HD11	1.99	0.44
1:B:323:ILE:HD11	1:B:327:VAL:HG21	1.99	0.44
1:B:335:ARG:HH12	1:B:405:LEU:HD11	1.83	0.44
1:A:147:PRO:HB3	1:A:165:HIS:HA	2.00	0.44
1:B:335:ARG:HH12	1:B:405:LEU:CD1	2.30	0.44
1:B:339:ILE:CG2	1:B:365:ASP:H	2.31	0.44
1:A:133:GLN:HG3	1:B:70:LYS:HG2	1.99	0.44
1:B:298:LYS:NZ	1:B:325:GLY:O	2.37	0.43
1:A:348:TRP:CE3	1:A:380:LEU:HD21	2.54	0.43
1:B:339:ILE:HD11	1:B:342:PHE:CD2	2.53	0.43
1:B:128:PHE:CD2	1:B:191:ILE:HD11	2.54	0.43
1:B:57:ASP:HB3	1:B:60:VAL:HG22	2.01	0.43
1:B:236:ILE:HD13	1:B:299:PHE:HE2	1.84	0.42
1:A:13:GLU:HG2	1:A:304:TRP:CD1	2.54	0.42
1:B:33:ILE:HG21	1:B:61:MSE:HE1	2.00	0.42
1:A:291:ILE:HA	1:A:294:MSE:HE2	2.01	0.42
1:A:332:LEU:HD12	1:A:378:ALA:HB3	2.01	0.42
1:B:68:ILE:HG22	1:B:74:ILE:HD11	2.02	0.42
1:A:296:GLU:HG2	1:A:301:ILE:O	2.20	0.41
1:B:335:ARG:NH1	1:B:405:LEU:HD11	2.35	0.41
1:B:144:LEU:O	1:B:194:LYS:HE2	2.21	0.41
1:A:196:ILE:HG13	1:A:196:ILE:O	2.21	0.41
1:B:200:GLU:OE2	1:B:268:GLU:HB3	2.21	0.41
1:B:339:ILE:HG22	1:B:365:ASP:H	1.86	0.40
1:A:292:SER:O	1:A:296:GLU:HG3	2.21	0.40
1:B:62:LYS:HD2	1:B:94:TYR:CZ	2.57	0.40

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	382/413 (92%)	373 (98%)	9 (2%)	0	100	100
1	B	382/413 (92%)	375 (98%)	7 (2%)	0	100	100
All	All	764/826 (92%)	748 (98%)	16 (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	340/350 (97%)	337 (99%)	3 (1%)	84	96
1	B	340/350 (97%)	340 (100%)	0	100	100
All	All	680/700 (97%)	677 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	VAL
1	A	197	GLU
1	A	198	MSE

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

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [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	378/413 (91%)	0.21	24 (6%) 23 14	13, 38, 79, 99	0
1	B	378/413 (91%)	0.23	30 (7%) 15 8	11, 36, 90, 116	0
All	All	756/826 (91%)	0.22	54 (7%) 19 10	11, 37, 83, 116	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	366	VAL	5.4
1	B	335	ARG	4.2
1	A	336	ASN	3.6
1	B	364	GLY	3.5
1	A	171	GLU	3.5
1	A	197	GLU	3.5
1	A	196	ILE	3.4
1	B	404	HIS	3.3
1	A	195	CYS	3.3
1	B	361	TYR	3.2
1	B	336	ASN	3.2
1	A	176	THR	3.2
1	B	399	GLN	3.1
1	A	159	LEU	3.0
1	B	400	THR	3.0
1	B	362	GLN	2.9
1	A	334	CYS	2.9
1	B	176	THR	2.9
1	B	363	GLU	2.8
1	A	335	ARG	2.8
1	B	401	TYR	2.7
1	B	403	LEU	2.7
1	A	164	ILE	2.6
1	B	402	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	399	GLN	2.6
1	B	339	ILE	2.6
1	B	346	GLU	2.6
1	B	273	HIS	2.6
1	A	172	ASP	2.6
1	B	197	GLU	2.6
1	B	388	ASN	2.6
1	A	339	ILE	2.5
1	A	156	SER	2.5
1	B	319	THR	2.5
1	A	360	LEU	2.5
1	B	398	LYS	2.4
1	B	163	ILE	2.4
1	A	363	GLU	2.4
1	A	149	ILE	2.4
1	A	177	SER	2.3
1	B	340	LYS	2.3
1	B	317	ASN	2.3
1	A	142	GLU	2.3
1	A	272	THR	2.3
1	B	318	LEU	2.2
1	A	146	TRP	2.2
1	B	274	SER	2.1
1	B	367	VAL	2.1
1	A	340	LYS	2.1
1	B	376	ASP	2.1
1	A	271	ARG	2.1
1	B	332	LEU	2.0
1	A	338	THR	2.0
1	B	221	THR	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 ⓘ

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.