



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:30 pm GMT

PDB ID : 5BR9  
Title : Crystal structure of an uncharacterized protein with similarity to peptidase  
YEAZ from Pseudomonas aeruginosa  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2015-05-29  
Resolution : 2.35 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

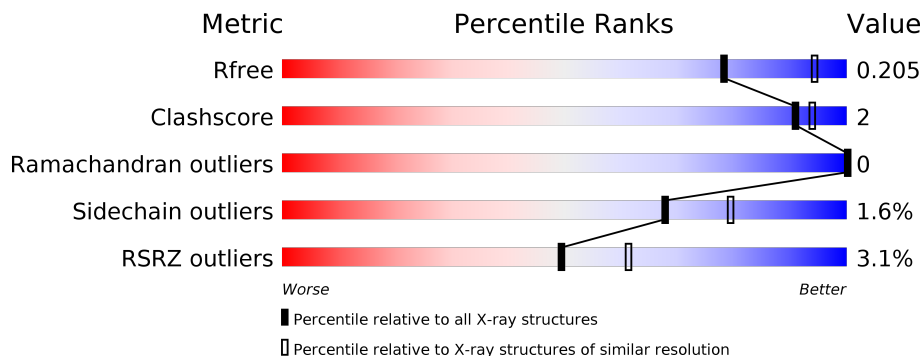
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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	234	<div> <div>86%</div> <div>6% 7%</div> </div>
1	B	234	<div> <div>88%</div> <div>8%</div> </div>
1	C	234	<div> <div>2%</div> <div>85%</div> <div>8% 7%</div> </div>
1	D	234	<div> <div>3%</div> <div>86%</div> <div>5% 9%</div> </div>
1	E	234	<div> <div>9%</div> <div>87%</div> <div>5% 8%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8442 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	3	0
			1637	1039	292	299	7			
1	B	216	Total	C	N	O	S	0	3	0
			1614	1028	288	292	6			
1	C	218	Total	C	N	O	S	0	4	0
			1645	1047	294	297	7			
1	D	214	Total	C	N	O	S	0	5	0
			1603	1022	287	288	6			
1	E	216	Total	C	N	O	S	0	3	0
			1559	995	271	286	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q9H XV5
A	-6	ALA	-	expression tag	UNP Q9H XV5
A	-5	HIS	-	expression tag	UNP Q9H XV5
A	-4	HIS	-	expression tag	UNP Q9H XV5
A	-3	HIS	-	expression tag	UNP Q9H XV5
A	-2	HIS	-	expression tag	UNP Q9H XV5
A	-1	HIS	-	expression tag	UNP Q9H XV5
A	0	HIS	-	expression tag	UNP Q9H XV5
B	-7	MET	-	expression tag	UNP Q9H XV5
B	-6	ALA	-	expression tag	UNP Q9H XV5
B	-5	HIS	-	expression tag	UNP Q9H XV5
B	-4	HIS	-	expression tag	UNP Q9H XV5
B	-3	HIS	-	expression tag	UNP Q9H XV5
B	-2	HIS	-	expression tag	UNP Q9H XV5
B	-1	HIS	-	expression tag	UNP Q9H XV5
B	0	HIS	-	expression tag	UNP Q9H XV5
C	-7	MET	-	expression tag	UNP Q9H XV5
C	-6	ALA	-	expression tag	UNP Q9H XV5
C	-5	HIS	-	expression tag	UNP Q9H XV5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP Q9H XV5
C	-3	HIS	-	expression tag	UNP Q9H XV5
C	-2	HIS	-	expression tag	UNP Q9H XV5
C	-1	HIS	-	expression tag	UNP Q9H XV5
C	0	HIS	-	expression tag	UNP Q9H XV5
D	-7	MET	-	expression tag	UNP Q9H XV5
D	-6	ALA	-	expression tag	UNP Q9H XV5
D	-5	HIS	-	expression tag	UNP Q9H XV5
D	-4	HIS	-	expression tag	UNP Q9H XV5
D	-3	HIS	-	expression tag	UNP Q9H XV5
D	-2	HIS	-	expression tag	UNP Q9H XV5
D	-1	HIS	-	expression tag	UNP Q9H XV5
D	0	HIS	-	expression tag	UNP Q9H XV5
E	-7	MET	-	expression tag	UNP Q9H XV5
E	-6	ALA	-	expression tag	UNP Q9H XV5
E	-5	HIS	-	expression tag	UNP Q9H XV5
E	-4	HIS	-	expression tag	UNP Q9H XV5
E	-3	HIS	-	expression tag	UNP Q9H XV5
E	-2	HIS	-	expression tag	UNP Q9H XV5
E	-1	HIS	-	expression tag	UNP Q9H XV5
E	0	HIS	-	expression tag	UNP Q9H XV5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	115	Total	O	0	0
			115	115		
2	B	84	Total	O	0	0
			84	84		
2	C	104	Total	O	0	0
			104	104		
2	D	57	Total	O	0	0
			57	57		
2	E	24	Total	O	0	0
			24	24		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.35Å 201.94Å 162.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 2.35 48.22 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.22-2.35) 99.7 (48.22-2.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.161 , 0.206 0.160 , 0.205	Depositor DCC
$R_{free}$ test set	2767 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8442	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.42	0/1682	0.56	0/2296
1	B	0.40	0/1658	0.53	0/2265
1	C	0.41	0/1695	0.55	0/2315
1	D	0.39	0/1654	0.54	0/2262
1	E	0.30	0/1602	0.48	0/2196
All	All	0.39	0/8291	0.53	0/11334

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	1637	0	1614	6	0
1	B	1614	0	1595	6	0
1	C	1645	0	1613	10	0
1	D	1603	0	1578	7	0
1	E	1559	0	1495	5	0
2	A	115	0	0	1	0
2	B	84	0	0	1	0
2	C	104	0	0	0	0
2	D	57	0	0	0	0
2	E	24	0	0	0	0
All	All	8442	0	7895	32	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.

All (32) 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:B:90:VAL:HG21	1:B:210:ALA:HB2	1.78	0.64
1:B:216:ARG:NH2	2:B:302:HOH:O	2.31	0.64
1:A:211:LEU:HD12	1:A:212:PRO:HD2	1.82	0.61
1:E:90:VAL:HG21	1:E:210:ALA:HB2	1.86	0.56
1:D:64[B]:ARG:HD3	1:D:213:VAL:HB	1.90	0.53
1:C:90:VAL:HG21	1:C:210:ALA:HB2	1.91	0.51
1:E:95:ASP:HA	1:E:98:ILE:HD12	1.92	0.50
1:C:12:GLU:HG3	1:C:30:VAL:HG13	1.96	0.48
1:C:15:SER:HA	1:C:42:MET:HE1	1.97	0.47
1:A:66:PRO:HB2	1:A:124:TYR:CD2	2.51	0.46
1:D:90:VAL:HG21	1:D:210:ALA:HB2	1.97	0.46
1:A:16:VAL:HG23	1:A:46:LEU:HD22	1.98	0.45
1:B:134:GLU:CD	1:B:136:ARG:HD3	2.36	0.45
1:D:64[B]:ARG:NH1	1:D:213:VAL:HG11	2.31	0.45
1:B:40:LEU:HD11	1:C:80:GLN:HB3	2.00	0.44
1:E:134:GLU:CD	1:E:136:ARG:HD3	2.38	0.44
1:C:115:ALA:HA	1:C:124:TYR:O	2.18	0.43
1:C:171:GLU:OE2	1:D:111:ARG:NH2	2.39	0.43
1:C:80:GLN:HG2	1:C:207:ALA:O	2.19	0.43
1:B:38:ARG:HA	1:B:38:ARG:HD2	1.85	0.43
1:C:16:VAL:HG23	1:C:46:LEU:HD22	2.01	0.43
1:A:125:TRP:CE2	1:A:149:VAL:HB	2.53	0.43
1:B:7:LEU:HD22	1:B:16:VAL:HG12	2.01	0.42
1:D:134:GLU:CD	1:D:136:ARG:HD3	2.40	0.42
1:D:7:LEU:HD12	1:D:79:VAL:HG22	2.01	0.42
1:C:38:ARG:C	1:C:41:PRO:HD2	2.40	0.41
1:E:70:THR:O	1:E:74:ILE:HG13	2.21	0.41
1:D:102:ARG:NH1	1:D:185:LEU:O	2.52	0.41
1:A:165:THR:HA	1:A:182:ALA:O	2.20	0.41
1:C:62:PHE:HB3	1:C:79:VAL:HG21	2.02	0.41
1:A:44[B]:ARG:NH1	2:A:301:HOH:O	2.25	0.40
1:E:58:ASP:O	1:E:89:PRO:HD2	2.21	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	218/234 (93%)	216 (99%)	2 (1%)	0	100	100
1	B	217/234 (93%)	213 (98%)	4 (2%)	0	100	100
1	C	220/234 (94%)	216 (98%)	4 (2%)	0	100	100
1	D	217/234 (93%)	213 (98%)	4 (2%)	0	100	100
1	E	217/234 (93%)	214 (99%)	3 (1%)	0	100	100
All	All	1089/1170 (93%)	1072 (98%)	17 (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	157/173 (91%)	153 (98%)	4 (2%)	53	66
1	B	153/173 (88%)	152 (99%)	1 (1%)	87	93
1	C	156/173 (90%)	153 (98%)	3 (2%)	62	75
1	D	150/173 (87%)	146 (97%)	4 (3%)	50	63
1	E	140/173 (81%)	138 (99%)	2 (1%)	71	82
All	All	756/865 (87%)	742 (98%)	14 (2%)	68	75

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	31	ILE
1	A	37	GLN
1	A	38	ARG
1	B	31	ILE
1	C	153[A]	TRP
1	C	153[B]	TRP
1	C	178	VAL
1	D	148	ARG
1	D	153[A]	TRP
1	D	153[B]	TRP
1	D	213	VAL
1	E	132	GLN
1	E	216	ARG

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 ⓘ

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	217/234 (92%)	-0.07	0 100 100	21, 32, 62, 94	0
1	B	216/234 (92%)	-0.37	1 (0%) 90 95	23, 38, 71, 109	0
1	C	218/234 (93%)	-0.20	4 (1%) 69 78	21, 36, 71, 103	0
1	D	214/234 (91%)	-0.07	7 (3%) 47 59	26, 44, 81, 121	0
1	E	216/234 (92%)	0.44	21 (9%) 8 13	28, 64, 102, 125	0
All	All	1081/1170 (92%)	-0.05	33 (3%) 49 61	21, 40, 87, 125	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	ALA	5.8
1	E	46	LEU	5.3
1	E	36	ALA	4.5
1	E	19	LEU	4.2
1	C	155	ALA	4.0
1	E	155	ALA	3.8
1	D	69	PHE	3.8
1	E	22	GLY	3.6
1	E	24	ALA	3.4
1	E	18	LEU	3.3
1	D	71	GLY	3.2
1	D	214	TYR	3.0
1	E	23	ARG	2.9
1	E	20	HIS	2.9
1	E	104	TYR	2.8
1	E	1	MET	2.7
1	E	3	THR	2.6
1	E	157	ALA	2.6
1	B	155	ALA	2.5
1	D	70	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	11	THR	2.4
1	E	59	ALA	2.4
1	E	51	GLY	2.3
1	E	109	ALA	2.3
1	C	157	ALA	2.3
1	C	216	ARG	2.2
1	E	178	VAL	2.2
1	E	56	ALA	2.2
1	E	199	TRP	2.1
1	C	156	ALA	2.1
1	E	192	LEU	2.1
1	D	36	ALA	2.1
1	E	179	ALA	2.1

## 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.