



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 11:33 am GMT

PDB ID : 2A5L  
Title : The crystal structure of the Trp repressor binding protein WrbA from *Pseudomonas aeruginosa*  
Authors : Lunin, V.V.; Evdokimova, E.; Kudritska, M.; Osipiuk, J.; Joachimiak, A.; Edwards, A.M.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2005-06-30  
Resolution : 1.70 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

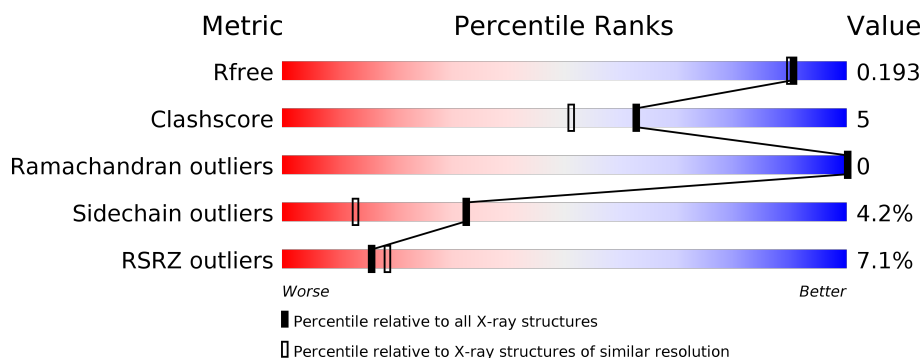
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	111664	3793 (1.70-1.70)
Clashscore	122126	4167 (1.70-1.70)
Ramachandran outliers	120053	4100 (1.70-1.70)
Sidechain outliers	120020	4100 (1.70-1.70)
RSRZ outliers	108989	3718 (1.70-1.70)

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	200	<div> <div>4%</div> <div>80%</div> <div>6% •</div> <div>15%</div> </div>
1	B	200	<div> <div>9%</div> <div>75%</div> <div>11% ••</div> <div>13%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3132 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 Trp repressor binding protein WrbA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	Se	0	4	0
			1305	828	229	242	2	4			
1	B	175	Total	C	N	O	S	Se	0	6	0
			1348	852	235	255	2	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	GB 15596146
A	0	SER	-	CLONING ARTIFACT	GB 15596146
A	1	MSE	MET	MODIFIED RESIDUE	GB 15596146
A	20	MSE	MET	MODIFIED RESIDUE	GB 15596146
A	84	MSE	MET	MODIFIED RESIDUE	GB 15596146
A	129	MSE	MET	MODIFIED RESIDUE	GB 15596146
A	138	MSE	MET	MODIFIED RESIDUE	GB 15596146
B	-1	GLY	-	CLONING ARTIFACT	GB 15596146
B	0	SER	-	CLONING ARTIFACT	GB 15596146
B	1	MSE	MET	MODIFIED RESIDUE	GB 15596146
B	20	MSE	MET	MODIFIED RESIDUE	GB 15596146
B	84	MSE	MET	MODIFIED RESIDUE	GB 15596146
B	129	MSE	MET	MODIFIED RESIDUE	GB 15596146
B	138	MSE	MET	MODIFIED RESIDUE	GB 15596146

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

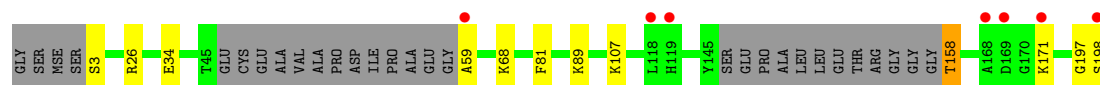
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	240	Total 240	O 240	0	0
3	B	237	Total 237	O 237	0	0

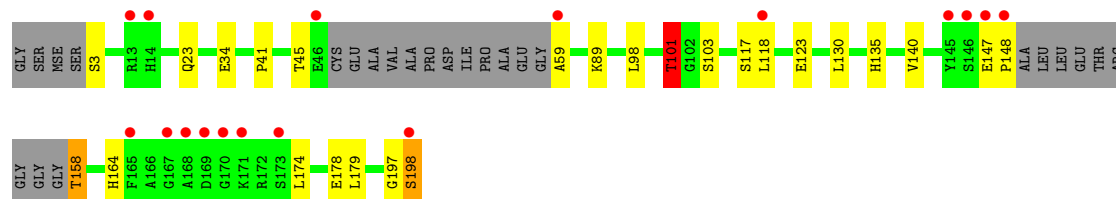
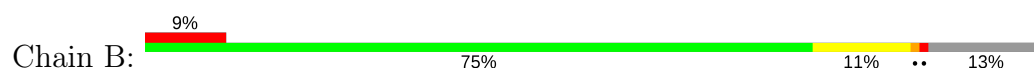
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Trp repressor binding protein WrbA



- Molecule 1: Trp repressor binding protein WrbA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.93Å 62.93Å 190.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.90 – 1.70 36.41 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.90-1.70) 99.8 (36.41-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.99 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.158 , 0.196 0.158 , 0.193	Depositor DCC
$R_{free}$ test set	2174 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 69.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.75	0/1327	0.78	0/1788
1	B	0.75	1/1371 (0.1%)	0.83	3/1848 (0.2%)
All	All	0.75	1/2698 (0.0%)	0.80	3/3636 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	123	GLU	CB-CG	-5.58	1.41	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	THR	N-CA-CB	-5.66	99.55	110.30
1	B	98	LEU	CB-CG-CD2	5.35	120.10	111.00
1	B	101	THR	OG1-CB-CG2	5.22	122.01	110.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	45	THR	Peptide

## 5.2 Too-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 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	1305	0	1311	9	0
1	B	1348	0	1335	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	240	0	0	3	0
3	B	237	0	0	6	0
All	All	3132	0	2646	25	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 5.

All (25) 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:34[A]:GLU:OE1	3:B:424:HOH:O	2.04	0.75
1:A:81:PHE:HD1	1:B:135[B]:HIS:HD2	1.38	0.71
1:B:174:LEU:HD22	1:B:178:GLU:HB3	1.75	0.68
1:A:59:ALA:N	3:A:428:HOH:O	2.26	0.67
1:A:81:PHE:CD1	1:B:135[B]:HIS:HD2	2.11	0.67
1:A:81:PHE:HD1	1:B:135[B]:HIS:CD2	2.14	0.65
1:A:81:PHE:CD1	1:B:135[B]:HIS:CD2	2.84	0.64
1:B:164:HIS:CD2	1:B:174:LEU:HD23	2.37	0.60
1:B:59:ALA:HB1	3:B:334:HOH:O	2.02	0.59
1:A:197:GLY:O	1:A:198:SER:HB2	2.01	0.58
1:B:101:THR:HG23	1:B:103:SER:OG	2.04	0.57
1:B:101:THR:CG2	1:B:103:SER:OG	2.53	0.56
1:B:197:GLY:O	1:B:198:SER:HB2	2.06	0.55
1:B:59:ALA:HB3	3:B:404:HOH:O	2.07	0.55
1:B:101:THR:HG21	3:B:257:HOH:O	2.11	0.51
1:A:34:GLU:HG3	3:A:427:HOH:O	2.12	0.50
1:A:158:THR:N	3:A:317:HOH:O	2.47	0.48
1:B:130:LEU:HD22	1:B:140:VAL:CG1	2.46	0.46
1:B:41:PRO:HD3	3:B:238:HOH:O	2.16	0.45
1:B:130:LEU:HD22	1:B:140:VAL:HG13	1.99	0.44
1:B:158:THR:N	3:B:426:HOH:O	2.51	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:SER:HB2	1:B:34[B]:GLU:OE1	2.19	0.43
1:B:23:GLN:HG3	1:B:179:LEU:HD23	2.02	0.42
1:A:68:LYS:O	1:A:107:LYS:NZ	2.53	0.42
1:B:147:GLU:O	1:B:148:PRO:C	2.58	0.41

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	169/200 (84%)	168 (99%)	1 (1%)	0	100	100
1	B	175/200 (88%)	173 (99%)	2 (1%)	0	100	100
All	All	344/400 (86%)	341 (99%)	3 (1%)	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	135/146 (92%)	130 (96%)	5 (4%)	37	16
1	B	139/146 (95%)	133 (96%)	6 (4%)	32	12
All	All	274/292 (94%)	263 (96%)	11 (4%)	32	14

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	26	ARG
1	A	89	LYS
1	A	158	THR
1	A	171	LYS
1	B	89	LYS
1	B	101	THR
1	B	117	SER
1	B	118	LEU
1	B	158	THR
1	B	198	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS

### 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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	167/200 (83%)	-0.08	7 (4%) 36 41	9, 14, 29, 39	0
1	B	171/200 (85%)	0.17	17 (9%) 7 8	10, 14, 35, 44	0
All	All	338/400 (84%)	0.05	24 (7%) 16 19	9, 14, 34, 44	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	118	LEU	6.2
1	B	148	PRO	6.0
1	A	198	SER	5.9
1	B	170	GLY	5.8
1	A	118	LEU	4.3
1	B	168	ALA	4.0
1	B	169	ASP	4.0
1	B	171	LYS	3.8
1	B	145	TYR	3.8
1	B	146	SER	3.6
1	A	168	ALA	3.5
1	B	59	ALA	3.5
1	A	119	HIS	3.4
1	B	198	SER	3.3
1	A	59	ALA	3.2
1	B	167	GLY	3.1
1	B	165	PHE	3.0
1	B	46	GLU	3.0
1	B	147	GLU	2.9
1	B	14	HIS	2.8
1	B	13	ARG	2.5
1	A	169	ASP	2.5
1	B	173	SER	2.3
1	A	171	LYS	2.2

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	199	1/1	0.92	0.25	22,22,22,22	1
2	MG	B	199	1/1	0.97	0.22	19,19,19,19	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.