



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 02:43 am BST

PDB ID : 3F79  
Title : Structure of pseudo-centered cell crystal form of the C-terminal phosphatase domain of *P. aeruginosa* RssB  
Authors : Levchenko, I.; Grant, R.A.; Sauer, R.T.; Baker, T.A.  
Deposited on : 2008-11-07  
Resolution : 2.80 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

<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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

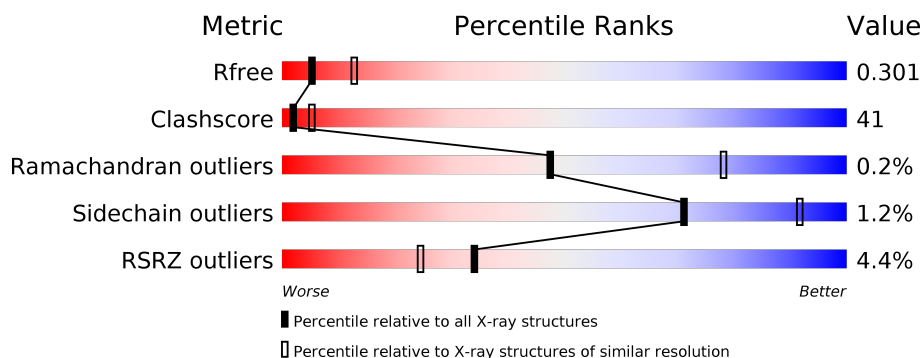
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 respectively. 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	255	<div> <div>5%</div> <div>41% 46% 13%</div> </div>
1	B	255	<div> <div>2%</div> <div>44% 45% 10%</div> </div>
1	C	255	<div> <div>5%</div> <div>38% 51% 10%</div> </div>
1	D	255	<div> <div>5%</div> <div>39% 50% 10%</div> </div>
1	E	255	<div> <div>4%</div> <div>52% 40% 7%</div> </div>
1	F	255	<div> <div>2%</div> <div>55% 37% 8%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10386 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 Probable two-component response regulator.

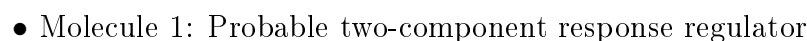
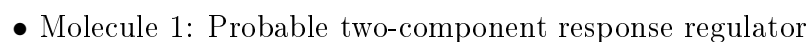
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	Se	12	0	0
			1659	1065	276	312	6			
1	B	229	Total	C	N	O	Se	5	0	0
			1738	1111	295	326	6			
1	C	229	Total	C	N	O	Se	5	0	0
			1728	1112	286	325	5			
1	D	230	Total	C	N	O	Se	0	0	0
			1719	1105	284	324	6			
1	E	236	Total	C	N	O	Se	13	0	0
			1778	1133	302	337	6			
1	F	235	Total	C	N	O	Se	12	0	0
			1757	1125	300	327	5			

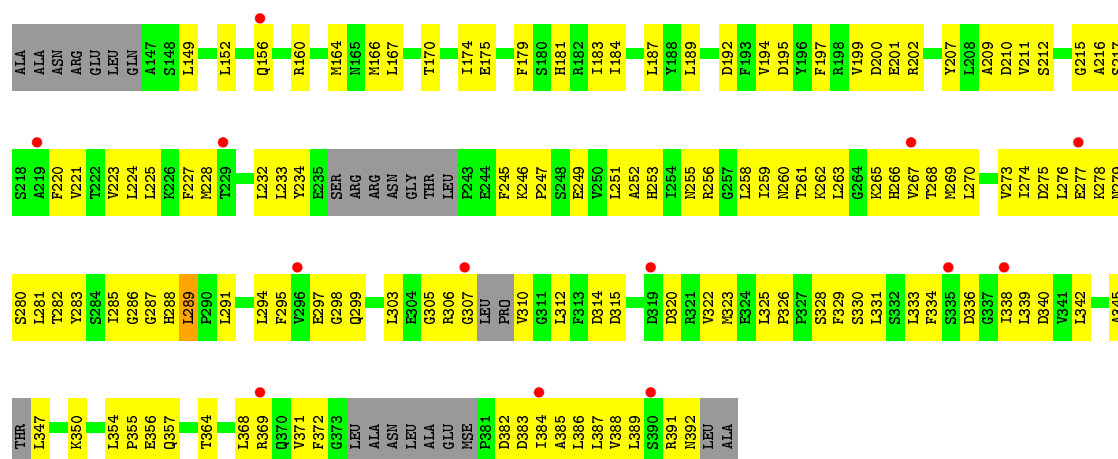
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	D	2	Total	Mg	0	0
			2	2		
2	C	1	Total	Mg	0	0
			1	1		
2	F	2	Total	Mg	0	0
			2	2		
2	E	1	Total	Mg	0	0
			1	1		

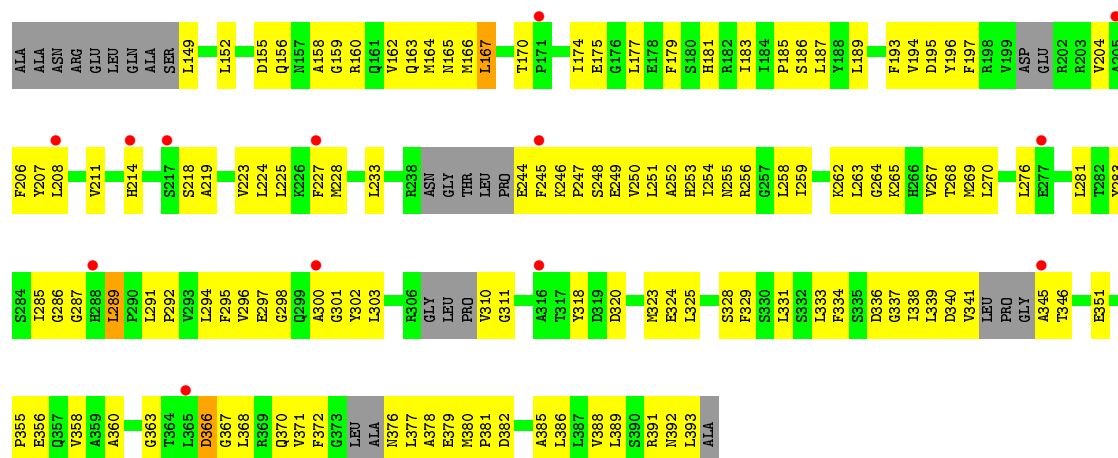


- Molecule 1: Probable two-component response regulator

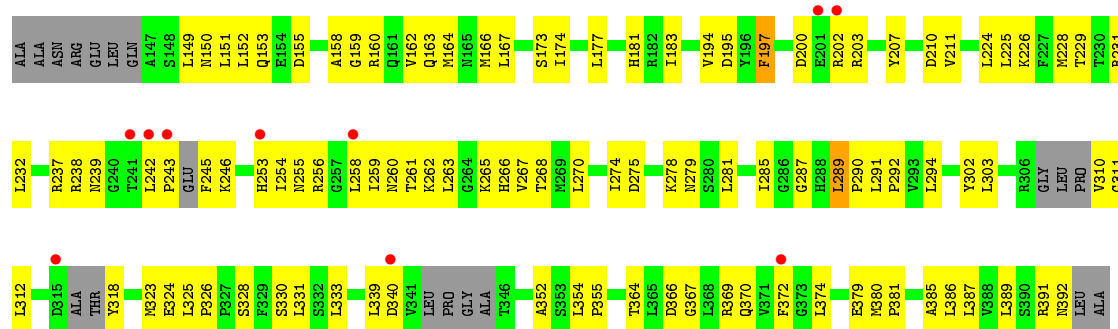




• Molecule 1: Probable two-component response regulator



• Molecule 1: Probable two-component response regulator



• Molecule 1: Probable two-component response regulator



ALA	ALA	ASN	ARG	GLU	LEU	GLN	A147	S148	L149	N150	L151	L152	Q153	E154	D155	Q156	N157	A158	G159	R160	Q161	V162	Q163	M164	M165	M166	L167	T170	I174	L177	H181	R182	I183	I184	P185	V194	D195	Y196	F197	R198	V199	D200	E201	R202	R203	V204	V211	S217	V221	T222	V223
L224	L225	K226	F227	N228	R231	L232	L233	R237	R238	R239	G240	THR	LEU	P243	E244	P245	K246	P247	V250	R256	I259	N260	T261	H266	V267	T268	M269	L270	V273	I274	E277	I285	G286	G287	R288	L289	P290	L291	P292	V293	L294	P295	Q299	A300	R306	GLY	LEU	P309			
V310	G311	L312	L325	S328	F329	S330	L331	S332	L333	F334	S335	D336	G337	I338	L339	I340	V341	L342	K350	L354	P355	T364	L365	D366	R369	Q370	V371	F372	GLY	LEU	ALA	ASN	LEU	ALA	GLU	NSE	P381	L384	A385	L386	L389	S390	R391	N392	L393	ALA					

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.87Å 124.87Å 92.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.80 37.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (15.00-2.80) 99.4 (37.41-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.243 , 0.297 0.244 , 0.301	Depositor DCC
$R_{free}$ test set	1983 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 58.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.047 for -h,-k,l 0.048 for h,-h-k,-l 0.477 for -k,-h,-l	Xtriage
Reported twinning fraction	0.498 for -k,-h,-l	Depositor
Outliers	0 of 39804 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	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 48.93 % 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 8.0149e-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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.21	0/1682	0.40	0/2271
1	B	0.24	0/1762	0.41	0/2371
1	C	0.23	0/1756	0.44	0/2374
1	D	0.26	0/1740	0.42	0/2349
1	E	0.22	0/1800	0.42	0/2429
1	F	0.24	0/1785	0.41	0/2413
All	All	0.23	0/10525	0.42	0/14207

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	1659	0	1613	128	0
1	B	1738	0	1706	165	0
1	C	1728	0	1687	193	0
1	D	1719	0	1680	190	0
1	E	1778	0	1758	119	0
1	F	1757	0	1713	121	0
2	B	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
All	All	10386	0	10157	842	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 41.

The worst 5 of 842 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:D:246:LYS:CB	1:D:249:GLU:HB3	1.35	1.51
1:D:246:LYS:HB2	1:D:249:GLU:CB	1.39	1.49
1:D:380:MSE:SE	1:D:381:PRO:HD2	1.85	1.26
1:B:356:GLU:HG3	1:B:357:GLN:NE2	1.56	1.20
1:D:175:GLU:O	1:D:391:ARG:NH2	1.73	1.19

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	209/255 (82%)	193 (92%)	16 (8%)	0	100	100
1	B	217/255 (85%)	202 (93%)	14 (6%)	1 (0%)	29	61
1	C	219/255 (86%)	199 (91%)	20 (9%)	0	100	100
1	D	218/255 (86%)	202 (93%)	15 (7%)	1 (0%)	29	61
1	E	226/255 (89%)	211 (93%)	15 (7%)	0	100	100
1	F	227/255 (89%)	214 (94%)	13 (6%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1316/1530 (86%)	1221 (93%)	93 (7%)	2 (0%)	47 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	310	VAL
1	D	337	GLY

### 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	173/206 (84%)	172 (99%)	1 (1%)	86 96
1	B	182/206 (88%)	179 (98%)	3 (2%)	62 88
1	C	181/206 (88%)	179 (99%)	2 (1%)	73 92
1	D	179/206 (87%)	175 (98%)	4 (2%)	52 83
1	E	189/206 (92%)	187 (99%)	2 (1%)	73 92
1	F	181/206 (88%)	180 (99%)	1 (1%)	86 96
All	All	1085/1236 (88%)	1072 (99%)	13 (1%)	71 92

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	289	LEU
1	D	167	LEU
1	E	197	PHE
1	C	187	LEU
1	D	376	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	253	HIS
1	C	266	HIS
1	E	163	GLN
1	C	163	GLN
1	D	376	ASN

### 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 7 ligands modelled in this entry, 7 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 [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	215/255 (84%)	0.17	13 (6%) 21 14	41, 92, 166, 244	0
1	B	222/255 (87%)	-0.12	6 (2%) 54 44	42, 86, 129, 224	0
1	C	223/255 (87%)	0.08	13 (5%) 23 15	43, 91, 141, 234	0
1	D	224/255 (87%)	0.04	13 (5%) 23 15	36, 88, 150, 275	0
1	E	228/255 (89%)	-0.04	10 (4%) 34 24	39, 86, 146, 192	0
1	F	228/255 (89%)	-0.19	4 (1%) 68 61	23, 80, 132, 226	0
All	All	1340/1530 (87%)	-0.01	59 (4%) 34 24	23, 88, 146, 275	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	GLY	6.1
1	B	288	HIS	5.8
1	C	369	ARG	5.7
1	A	238	ARG	5.5
1	A	185	PRO	5.4

### 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	F	4	1/1	0.79	0.19	94,94,94,94	0
2	MG	D	6	1/1	0.84	0.13	78,78,78,78	0
2	MG	F	3	1/1	0.84	0.09	47,47,47,47	0
2	MG	B	1	1/1	0.88	0.14	61,61,61,61	0
2	MG	C	5	1/1	0.94	0.17	50,50,50,50	0
2	MG	D	7	1/1	0.94	0.08	40,40,40,40	0
2	MG	E	2	1/1	0.96	0.11	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.