



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2020 – 02:08 PM JST

PDB ID : 7C1J  
Title : Crystal structure of the receiver domain of sensor histidine kinase PA1611 (PA1611REC) from *Pseudomonas aeruginosa* PAO1 with magnesium ion coordinated in the active site cleft  
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Deposited on : 2020-05-04  
Resolution : 1.35 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

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
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)	:	2.14.6

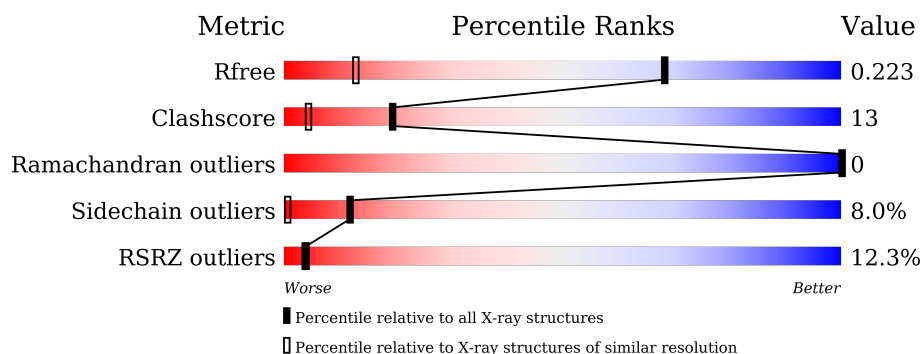
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 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))
$R_{free}$	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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 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	166	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1284 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 Histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	16	0
			1110	680	223	201	6			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	486	MET	-	initiating methionine	UNP A0A4U9SBT9
A	487	GLY	-	expression tag	UNP A0A4U9SBT9
A	488	SER	-	expression tag	UNP A0A4U9SBT9
A	489	SER	-	expression tag	UNP A0A4U9SBT9
A	490	HIS	-	expression tag	UNP A0A4U9SBT9
A	491	HIS	-	expression tag	UNP A0A4U9SBT9
A	492	HIS	-	expression tag	UNP A0A4U9SBT9
A	493	HIS	-	expression tag	UNP A0A4U9SBT9
A	494	HIS	-	expression tag	UNP A0A4U9SBT9
A	495	HIS	-	expression tag	UNP A0A4U9SBT9
A	496	SER	-	expression tag	UNP A0A4U9SBT9
A	497	SER	-	expression tag	UNP A0A4U9SBT9
A	498	GLY	-	expression tag	UNP A0A4U9SBT9
A	499	LEU	-	expression tag	UNP A0A4U9SBT9
A	500	VAL	-	expression tag	UNP A0A4U9SBT9
A	501	PRO	-	expression tag	UNP A0A4U9SBT9
A	502	ALA	-	expression tag	UNP A0A4U9SBT9
A	503	GLY	-	expression tag	UNP A0A4U9SBT9
A	504	SER	-	expression tag	UNP A0A4U9SBT9
A	505	HIS	-	expression tag	UNP A0A4U9SBT9
A	506	MET	-	expression tag	UNP A0A4U9SBT9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

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

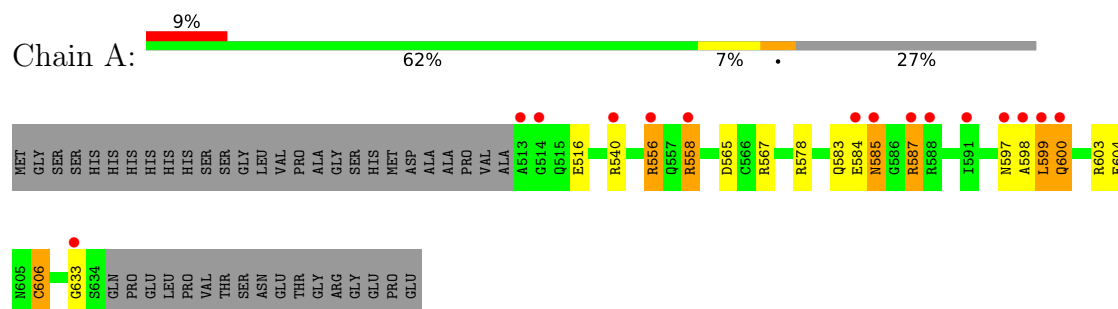
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	173	Total 173	O 173	0	0

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Histidine kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.96Å 57.96Å 67.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.16 – 1.35 20.15 – 1.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.16-1.35) 97.0 (20.15-1.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.180 , 0.216 0.190 , 0.223	Depositor DCC
$R_{free}$ test set	1448 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1284	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% 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](#)

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	0.78	0/1120	1.05	3/1505 (0.2%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	578[A]	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	578[B]	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	565	ASP	CB-CG-OD2	-5.09	113.72	118.30

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	1110	0	1127	29	0
2	A	1	0	0	0	0
3	A	173	0	0	13	3
All	All	1284	0	1127	29	3

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 13.

All (29) 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:603[A]:ARG:NH1	3:A:802:HOH:O	1.63	1.28
1:A:558[A]:ARG:HD2	1:A:585:ASN:HB3	1.58	0.86
1:A:603[A]:ARG:NE	3:A:803:HOH:O	2.10	0.84
1:A:597[A]:ASN:ND2	3:A:806:HOH:O	2.23	0.70
1:A:603[A]:ARG:NH2	3:A:807:HOH:O	2.25	0.70
1:A:558[A]:ARG:HD2	1:A:585:ASN:CB	2.21	0.69
1:A:583:GLN:O	1:A:587:ARG:HD2	1.94	0.67
1:A:600[A]:GLN:OE1	3:A:804:HOH:O	2.12	0.66
1:A:558[B]:ARG:HD3	1:A:558[B]:ARG:C	2.22	0.60
1:A:606:CYS:HB2	3:A:886:HOH:O	2.01	0.59
1:A:558[B]:ARG:HG3	1:A:558[B]:ARG:O	2.04	0.57
1:A:597[B]:ASN:C	1:A:599:LEU:H	2.08	0.55
1:A:597[A]:ASN:C	1:A:599:LEU:H	2.08	0.54
1:A:567:ARG:HD2	3:A:806:HOH:O	2.07	0.53
1:A:556[A]:ARG:NE	3:A:811:HOH:O	2.43	0.51
1:A:600[A]:GLN:NE2	3:A:804:HOH:O	2.42	0.51
1:A:558[B]:ARG:CG	1:A:558[B]:ARG:O	2.57	0.51
1:A:633:GLY:O	3:A:805:HOH:O	2.20	0.50
1:A:558[B]:ARG:CD	1:A:558[B]:ARG:C	2.79	0.49
1:A:585:ASN:N	1:A:585:ASN:HD22	2.10	0.49
1:A:598:ALA:O	1:A:603[B]:ARG:HD2	2.13	0.49
1:A:600[A]:GLN:CD	3:A:804:HOH:O	2.51	0.48
1:A:516:GLU:OE1	1:A:540:ARG:NE	2.44	0.47
1:A:585:ASN:N	1:A:585:ASN:ND2	2.63	0.46
1:A:599:LEU:H	1:A:599:LEU:HG	1.59	0.44
1:A:603[B]:ARG:NE	3:A:803:HOH:O	2.34	0.44
1:A:600[B]:GLN:NE2	1:A:604:GLU:OE1	2.37	0.42
1:A:585:ASN:HA	3:A:911:HOH:O	2.21	0.41
1:A:516:GLU:OE1	1:A:540:ARG:NH1	2.54	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:968:HOH:O	3:A:968:HOH:O[4_555]	1.62	0.58
3:A:809:HOH:O	3:A:814:HOH:O[4_555]	1.65	0.55
3:A:845:HOH:O	3:A:865:HOH:O[6_445]	1.92	0.28



## 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	136/166 (82%)	130 (96%)	6 (4%)	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	116/135 (86%)	105 (90%)	11 (10%)	8	0

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

Mol	Chain	Res	Type
1	A	556[A]	ARG
1	A	556[B]	ARG
1	A	558[A]	ARG
1	A	558[B]	ARG
1	A	584	GLU
1	A	585	ASN
1	A	587	ARG
1	A	599	LEU
1	A	600[A]	GLN
1	A	600[B]	GLN
1	A	606	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	549	GLN
1	A	585	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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	122/166 (73%)	0.87	15 (12%) <b>4</b> <b>4</b>	15, 21, 46, 69	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	ALA	8.7
1	A	585	ASN	5.3
1	A	599	LEU	5.3
1	A	633	GLY	4.5
1	A	584	GLU	4.1
1	A	514	GLY	3.2
1	A	587	ARG	3.0
1	A	598	ALA	2.9
1	A	600[A]	GLN	2.9
1	A	556[A]	ARG	2.7
1	A	588	ARG	2.7
1	A	597[A]	ASN	2.6
1	A	558[A]	ARG	2.5
1	A	591	ILE	2.3
1	A	540	ARG	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 monosaccharides in this entry.

## 6.4 Ligands

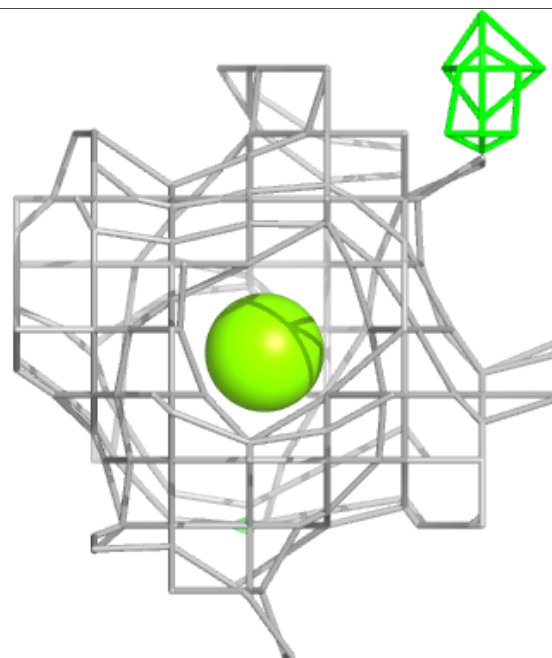
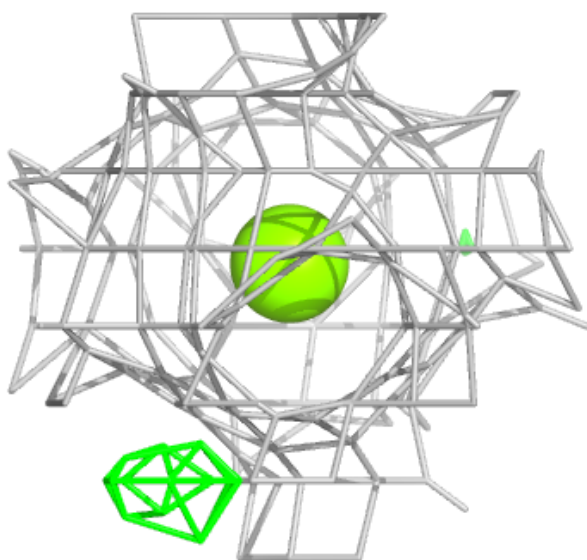
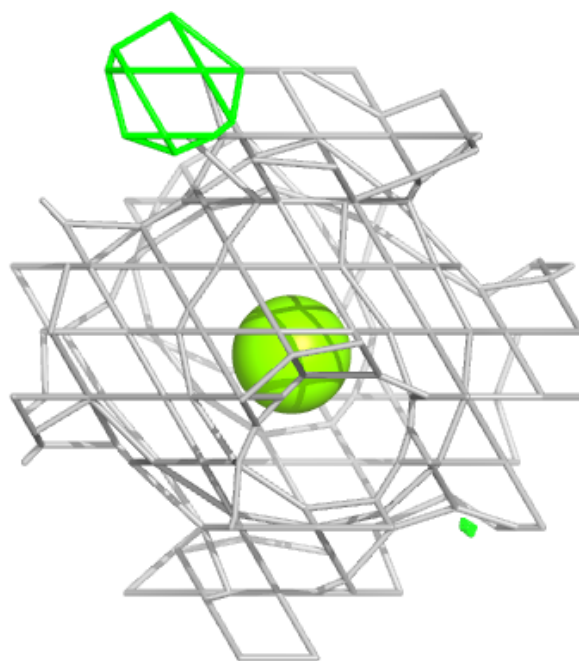
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	701	1/1	0.99	0.05	16,16,16,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around MG A 701:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.