



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2017 – 04:57 PM EST

PDB ID : 5MMH
Title : the X-Ray Structure of the Effector Domain of the Transcriptional Regulator
AmpR of Pseudomonas aeruginosa
Authors : Hermoso, J.A.; Dominguez gil Velasco, T.
Deposited on : 2016-12-09
Resolution : 2.20 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

A user guide is available at

<http://wwpdb.org/validation/2016/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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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-20028442

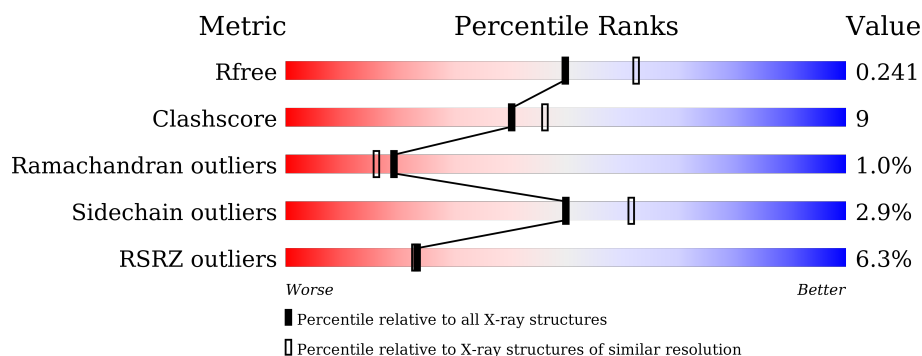
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 ≥ 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	222	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>5%</div> <div>7%</div> </div> </div>
1	B	222	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	222	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	222	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6818 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 HTH-type transcriptional activator AmpR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	1	0
			1605	1024	290	285	6			
1	B	201	Total	C	N	O	S	0	0	0
			1551	989	277	279	6			
1	C	203	Total	C	N	O	S	0	0	0
			1571	1003	281	281	6			
1	D	202	Total	C	N	O	S	0	2	0
			1585	1014	282	283	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	MET	-	initiating methionine	UNP P24734
A	297	LEU	-	expression tag	UNP P24734
A	298	GLU	-	expression tag	UNP P24734
A	299	HIS	-	expression tag	UNP P24734
A	300	HIS	-	expression tag	UNP P24734
A	301	HIS	-	expression tag	UNP P24734
A	302	HIS	-	expression tag	UNP P24734
A	303	HIS	-	expression tag	UNP P24734
A	304	HIS	-	expression tag	UNP P24734
B	83	MET	-	initiating methionine	UNP P24734
B	297	LEU	-	expression tag	UNP P24734
B	298	GLU	-	expression tag	UNP P24734
B	299	HIS	-	expression tag	UNP P24734
B	300	HIS	-	expression tag	UNP P24734
B	301	HIS	-	expression tag	UNP P24734
B	302	HIS	-	expression tag	UNP P24734
B	303	HIS	-	expression tag	UNP P24734
B	304	HIS	-	expression tag	UNP P24734
C	83	MET	-	initiating methionine	UNP P24734
C	297	LEU	-	expression tag	UNP P24734
C	298	GLU	-	expression tag	UNP P24734

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Chain	Residue	Modelled	Actual	Comment	Reference
C	299	HIS	-	expression tag	UNP P24734
C	300	HIS	-	expression tag	UNP P24734
C	301	HIS	-	expression tag	UNP P24734
C	302	HIS	-	expression tag	UNP P24734
C	303	HIS	-	expression tag	UNP P24734
C	304	HIS	-	expression tag	UNP P24734
D	83	MET	-	initiating methionine	UNP P24734
D	297	LEU	-	expression tag	UNP P24734
D	298	GLU	-	expression tag	UNP P24734
D	299	HIS	-	expression tag	UNP P24734
D	300	HIS	-	expression tag	UNP P24734
D	301	HIS	-	expression tag	UNP P24734
D	302	HIS	-	expression tag	UNP P24734
D	303	HIS	-	expression tag	UNP P24734
D	304	HIS	-	expression tag	UNP P24734

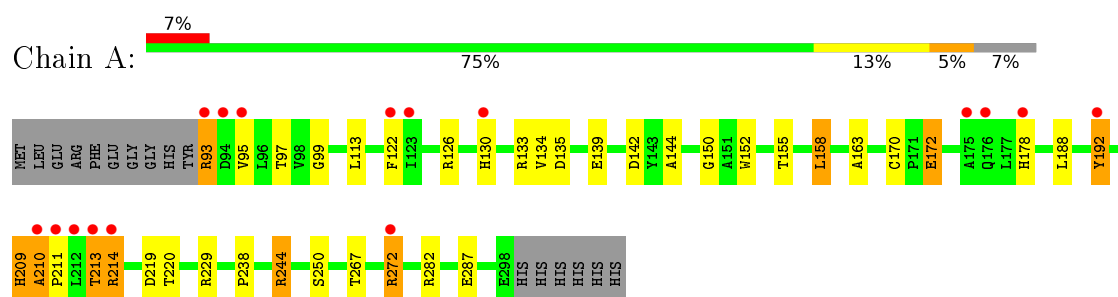
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	106	Total O 106 106	0	0
2	B	130	Total O 130 130	0	0
2	C	132	Total O 132 132	0	0
2	D	138	Total O 138 138	0	0

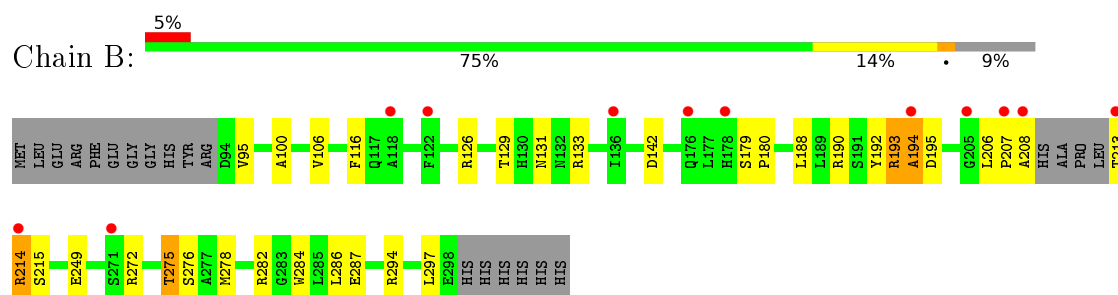
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

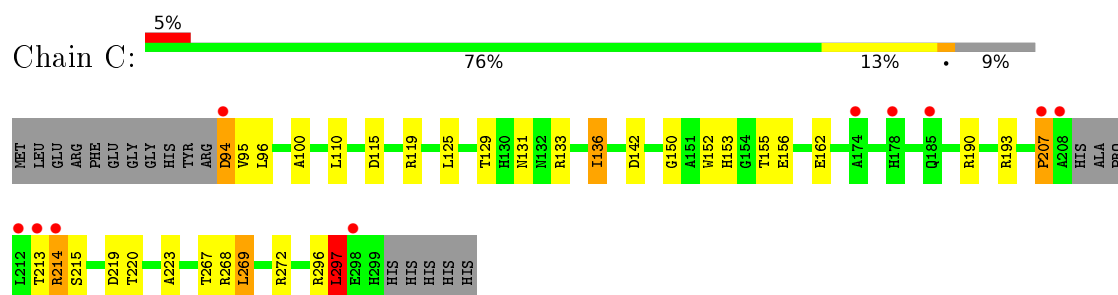
- Molecule 1: HTH-type transcriptional activator AmpR



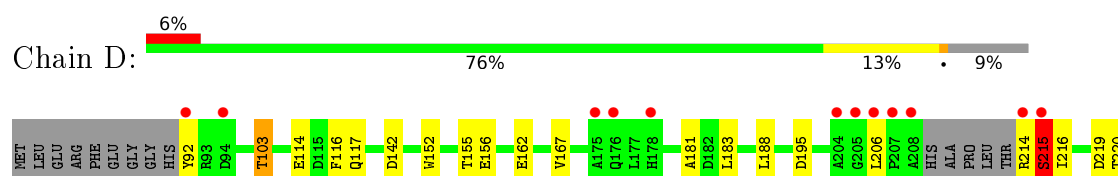
- Molecule 1: HTH-type transcriptional activator AmpR



- Molecule 1: HTH-type transcriptional activator AmpR



- Molecule 1: HTH-type transcriptional activator AmpR





4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.72Å 71.00Å 124.01Å 90.00° 112.62° 90.00°	Depositor
Resolution (Å)	35.38 – 2.20 35.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (35.38-2.20) 98.7 (35.38-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.194 , 0.242 0.192 , 0.241	Depositor DCC
R_{free} test set	2280 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6818	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 24.03 % 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 4.1509e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

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	0.45	0/1646	0.66	1/2243 (0.0%)
1	B	0.45	0/1588	0.62	1/2161 (0.0%)
1	C	0.53	4/1609 (0.2%)	0.68	3/2190 (0.1%)
1	D	0.44	0/1625	0.65	3/2212 (0.1%)
All	All	0.47	4/6468 (0.1%)	0.65	8/8806 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	190	ARG	CZ-NH2	-7.99	1.22	1.33
1	C	190	ARG	NE-CZ	-7.32	1.23	1.33
1	C	190	ARG	CZ-NH1	-6.13	1.25	1.33
1	C	190	ARG	CD-NE	-5.13	1.37	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	269	LEU	CB-CG-CD2	-9.66	94.58	111.00
1	C	136	ILE	CG1-CB-CG2	7.14	127.11	111.40
1	A	209	HIS	C-N-CA	5.84	136.31	121.70
1	D	219	ASP	CB-CG-OD1	5.61	123.34	118.30
1	B	193	ARG	C-N-CA	5.49	135.43	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	214	ARG	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	1605	0	1585	31	0
1	B	1551	0	1524	32	0
1	C	1571	0	1549	26	0
1	D	1585	0	1549	21	0
2	A	106	0	0	8	1
2	B	130	0	0	10	1
2	C	132	0	0	8	0
2	D	138	0	0	4	0
All	All	6818	0	6207	109	1

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 9.

The worst 5 of 109 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:287:GLU:OE2	2:A:401:HOH:O	1.87	0.93
1:B:190:ARG:NH2	1:B:215:SER:OG	2.04	0.91
1:B:275:THR:HG22	1:B:278:MET:H	1.39	0.87
1:C:110:LEU:O	2:C:401:HOH:O	1.91	0.85
1:C:193:ARG:NH2	2:C:404:HOH:O	2.02	0.84

All (1) 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)
2:A:463:HOH:O	2:B:455:HOH:O[1_545]	1.91	0.29

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	205/222 (92%)	198 (97%)	5 (2%)	2 (1%)	19	16
1	B	197/222 (89%)	187 (95%)	8 (4%)	2 (1%)	19	16
1	C	199/222 (90%)	190 (96%)	7 (4%)	2 (1%)	19	16
1	D	200/222 (90%)	192 (96%)	6 (3%)	2 (1%)	19	16
All	All	801/888 (90%)	767 (96%)	26 (3%)	8 (1%)	19	16

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	ALA
1	C	214	ARG
1	B	194	ALA
1	D	215	SER
1	D	216	ILE

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	160/173 (92%)	153 (96%)	7 (4%)	35	42
1	B	154/173 (89%)	150 (97%)	4 (3%)	54	66
1	C	157/173 (91%)	155 (99%)	2 (1%)	76	87
1	D	157/173 (91%)	152 (97%)	5 (3%)	46	57
All	All	628/692 (91%)	610 (97%)	18 (3%)	50	62

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	179	SER
1	B	275	THR
1	D	103	THR
1	A	272	ARG
1	B	106	VAL

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

Mol	Chain	Res	Type
1	C	270	GLN

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 [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, 95th 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 ²)	Q<0.9
1	A	206/222 (92%)	0.30	16 (7%) 16 15	13, 28, 51, 72	0
1	B	201/222 (90%)	0.41	12 (5%) 25 25	13, 28, 52, 76	0
1	C	203/222 (91%)	0.33	10 (4%) 33 33	11, 26, 51, 71	0
1	D	202/222 (90%)	0.26	13 (6%) 23 22	12, 25, 53, 68	0
All	All	812/888 (91%)	0.32	51 (6%) 23 23	11, 27, 52, 76	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	213	THR	7.6
1	B	213	THR	5.7
1	A	178	HIS	5.4
1	D	178	HIS	5.2
1	A	212	LEU	5.0

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.