



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 09:49 PM BST

PDB ID : 6IZH  
Title : Crystal structure of deaminase AmnE from Pseudomonas sp. AP-3  
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Deposited on : 2018-12-19  
Resolution : 1.75 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.

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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	:	2.13
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)	:	2.13

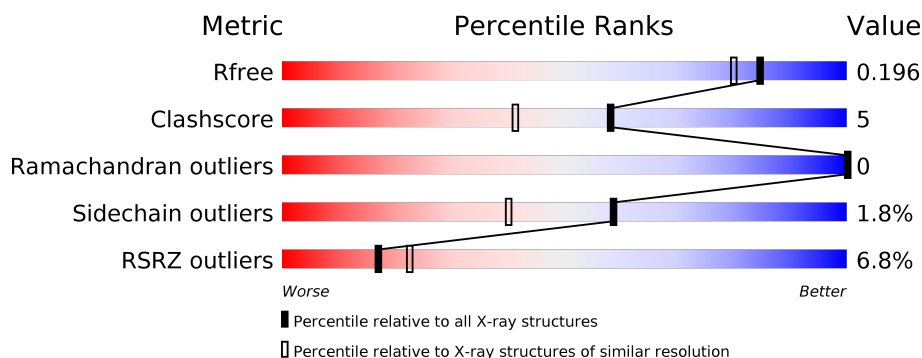
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	142	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>•</div> </div> </div>
1	B	142	<div> <div>9%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	C	142	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>• •</div> </div> </div>
1	D	142	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>•</div> </div> </div>
1	E	142	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>6%</div> <div>•</div> <div>15%</div> </div> </div>
1	F	142	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	142	<div><div></div><div>13%</div><div>75%</div><div>20%</div><div>• 5%</div></div>
1	H	142	<div><div></div><div>13%</div><div>82%</div><div>12%</div><div>• 5%</div></div>
1	I	142	<div><div></div><div>8%</div><div>82%</div><div>13%</div><div>• •</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10572 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 2-aminomuconate deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	3	0
			1086	685	193	205	3			
1	B	135	Total	C	N	O	S	0	4	0
			1079	682	193	201	3			
1	C	138	Total	C	N	O	S	0	5	0
			1103	696	195	208	4			
1	D	137	Total	C	N	O	S	0	6	0
			1100	692	194	210	4			
1	E	121	Total	C	N	O	S	0	4	0
			982	620	176	184	2			
1	F	137	Total	C	N	O	S	0	2	0
			1072	678	191	200	3			
1	G	135	Total	C	N	O	S	0	2	0
			1060	670	189	198	3			
1	H	135	Total	C	N	O	S	0	1	0
			1045	662	185	195	3			
1	I	136	Total	C	N	O	S	0	2	0
			1063	672	189	199	3			

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	101	Total 101	O 101	0	0
3	C	146	Total 146	O 146	0	0
3	D	132	Total 132	O 132	0	0
3	E	143	Total 143	O 143	0	0
3	F	124	Total 124	O 124	0	0
3	G	67	Total 67	O 67	0	0
3	H	88	Total 88	O 88	0	0
3	I	67	Total 67	O 67	0	0



- Molecule 1: 2-aminomuconate deaminase

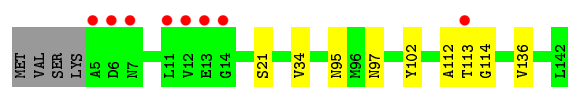


Figure 1 illustrates the structure of the 2019-2020 season. The top row shows the months from MET to DEC. The bottom row shows the corresponding months from JAN to DEC. Red dots indicate the months when the season was active: MET, VAL, SER, LYS, ALA, ASP, ASN, S8, A9, K10, L11, L12, E13, G14, K15, A16, K17, P18, M19, G20, P23, V34, R41, P42, E50, P51, D74, K104, V136, and L140.

Amino Acid	Number of Mutations
MET	0
VAL	0
SER	0
LYS	0
A5	3
D6	2
N7	1
M19	0
R41	0
P42	0
T45	0
D53	1
D82	0
Y102	0
N103	0
K104	0
D111	0
L142	0

Relative abundance of amino acids in the protein. The y-axis represents relative abundance from 0 to 1.0. The x-axis lists amino acids: MET, VAL, SER, LYS, ALA, D6, N7, M19, G20, S21, A28, R73, N95, M96, N97, Y102, N103, H127, and L142. Bars are colored in a repeating pattern of grey, green, yellow, and red. MET, VAL, SER, LYS, and ALA are grey. D6, N7, M19, G20, S21, A28, R73, N95, M96, N97, Y102, N103, H127, and L142 are green. The bars for D6 and N7 are significantly higher than the others, reaching approximately 0.85 and 0.80 respectively, and are marked with red dots above them.

MET VAL SER LYS ALA ASP ASN SER ALA LYS LEU VAL GLU GLY LYS ALA LYS PRO MET GLY P22 D43 N44 E50 P51 D52 D53 T54 G55 R56 Y102 K135 L142



WORLD WIDE  
PDB  
PROTEIN DATA BANK



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.87Å 54.78Å 134.59Å 90.00° 101.89° 90.00°	Depositor
Resolution (Å)	49.51 – 1.75 49.51 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.51-1.75) 98.6 (49.51-1.75)	Depositor EDS
$R_{merge}$	0.90	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.157 , 0.195 0.160 , 0.196	Depositor DCC
$R_{free}$ test set	5840 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.6	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	0.97	EDS
Total number of atoms	10572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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	0.37	0/1109	0.57	0/1508
1	B	0.34	0/1102	0.52	0/1495
1	C	0.36	0/1126	0.51	0/1531
1	D	0.37	0/1123	0.52	0/1526
1	E	0.37	0/1004	0.51	0/1369
1	F	0.36	0/1095	0.53	0/1488
1	G	0.29	0/1083	0.48	0/1472
1	H	0.31	0/1068	0.46	0/1453
1	I	0.29	0/1086	0.46	0/1475
All	All	0.34	0/9796	0.51	0/13317

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	1086	0	1075	11	0
1	B	1079	0	1078	6	0
1	C	1103	0	1090	9	0
1	D	1100	0	1082	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	982	0	966	6	0
1	F	1072	0	1063	10	0
1	G	1060	0	1051	23	0
1	H	1045	0	1035	14	0
1	I	1063	0	1052	16	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	A	112	0	0	3	0
3	B	101	0	0	0	0
3	C	146	0	0	3	0
3	D	132	0	0	1	0
3	E	143	0	0	2	0
3	F	124	0	0	3	0
3	G	67	0	0	0	0
3	H	88	0	0	1	0
3	I	67	0	0	1	0
All	All	10572	0	9492	92	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.

The worst 5 of 92 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:G:12:VAL:HG12	1:G:13:GLU:HB2	1.44	0.99
1:G:17:LYS:HD3	1:G:18:PRO:HD2	1.50	0.92
1:F:73[B]:ARG:NH1	3:F:201:HOH:O	2.04	0.91
1:I:73[B]:ARG:HH11	1:I:73[B]:ARG:HG2	1.37	0.88
1:A:112:ALA:HB3	1:A:113:THR:OG1	1.75	0.85

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	139/142 (98%)	132 (95%)	7 (5%)	0	100	100
1	B	137/142 (96%)	132 (96%)	5 (4%)	0	100	100
1	C	141/142 (99%)	138 (98%)	3 (2%)	0	100	100
1	D	141/142 (99%)	137 (97%)	4 (3%)	0	100	100
1	E	123/142 (87%)	121 (98%)	2 (2%)	0	100	100
1	F	137/142 (96%)	134 (98%)	3 (2%)	0	100	100
1	G	135/142 (95%)	126 (93%)	9 (7%)	0	100	100
1	H	134/142 (94%)	130 (97%)	4 (3%)	0	100	100
1	I	136/142 (96%)	131 (96%)	5 (4%)	0	100	100
All	All	1223/1278 (96%)	1181 (97%)	42 (3%)	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	118/120 (98%)	117 (99%)	1 (1%)	81	72
1	B	118/120 (98%)	116 (98%)	2 (2%)	60	42
1	C	120/120 (100%)	118 (98%)	2 (2%)	60	42
1	D	121/120 (101%)	119 (98%)	2 (2%)	60	42
1	E	108/120 (90%)	106 (98%)	2 (2%)	57	37
1	F	116/120 (97%)	114 (98%)	2 (2%)	60	42
1	G	115/120 (96%)	113 (98%)	2 (2%)	60	42
1	H	113/120 (94%)	109 (96%)	4 (4%)	36	13
1	I	116/120 (97%)	114 (98%)	2 (2%)	60	42
All	All	1045/1080 (97%)	1026 (98%)	19 (2%)	59	40

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	135	LYS
1	F	102	TYR
1	H	96	MET
1	E	102	TYR
1	H	102	TYR

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 monosaccharides 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 [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	138/142 (97%)	0.17	8 (5%) 23 28	16, 23, 48, 84	0
1	B	135/142 (95%)	0.50	13 (9%) 8 10	16, 23, 72, 115	0
1	C	138/142 (97%)	0.01	4 (2%) 51 57	15, 21, 41, 66	0
1	D	137/142 (96%)	-0.12	2 (1%) 73 80	16, 20, 40, 80	0
1	E	121/142 (85%)	0.00	2 (1%) 70 77	15, 20, 36, 63	0
1	F	137/142 (96%)	-0.03	3 (2%) 62 69	15, 22, 47, 67	0
1	G	135/142 (95%)	0.70	19 (14%) 2 4	19, 33, 88, 128	0
1	H	135/142 (95%)	0.72	19 (14%) 2 4	19, 30, 94, 130	0
1	I	136/142 (95%)	0.39	12 (8%) 10 13	19, 31, 67, 97	0
All	All	1212/1278 (94%)	0.26	82 (6%) 17 22	15, 24, 60, 130	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	GLY	9.8
1	B	11	LEU	9.7
1	H	11	LEU	9.1
1	A	5	ALA	8.8
1	G	11	LEU	8.7

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	MG	C	201	1/1	0.99	0.04	18,18,18,18	1
2	MG	E	201	1/1	1.00	0.07	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.