



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 03:17 am GMT

PDB ID : 2VI7  
Title : Structure of a Putative Acetyltransferase (PA1377) from *Pseudomonas aeruginosa*  
Authors : Davies, A.M.; Tata, R.; Chauviac, F.X.; Sutton, B.J.; Brown, P.R.  
Deposited on : 2007-11-28  
Resolution : 2.25 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

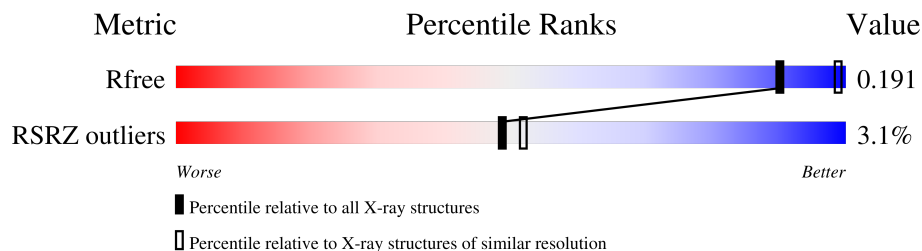
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1171	-	X	-	-
2	GOL	B	1170	-	X	-	-
2	GOL	C	1171	-	X	-	-
2	GOL	C	1172	-	X	-	-
2	GOL	C	1173	-	X	-	-

## 2 Entry composition [i](#)

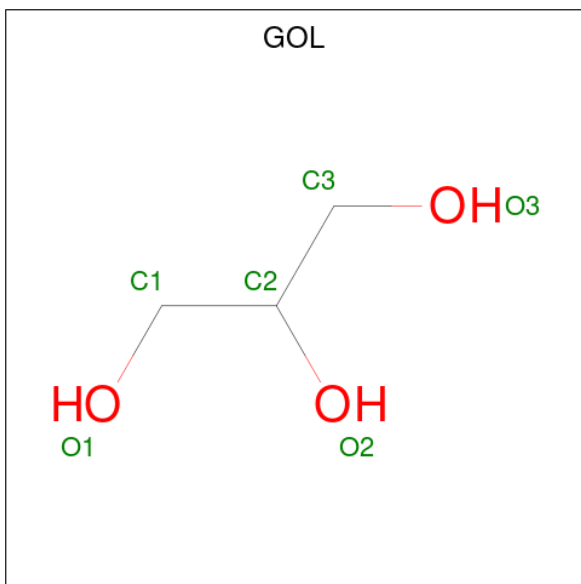
There are 5 unique types of molecules in this entry. The entry contains 4180 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLTRANSFERASE PA1377.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	163	Total 1274	C 801	N 239	O 229	S 5	0	2	0
1	B	163	Total 1274	C 801	N 236	O 232	S 5	0	1	0
1	C	165	Total 1295	C 810	N 251	O 229	S 5	0	1	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



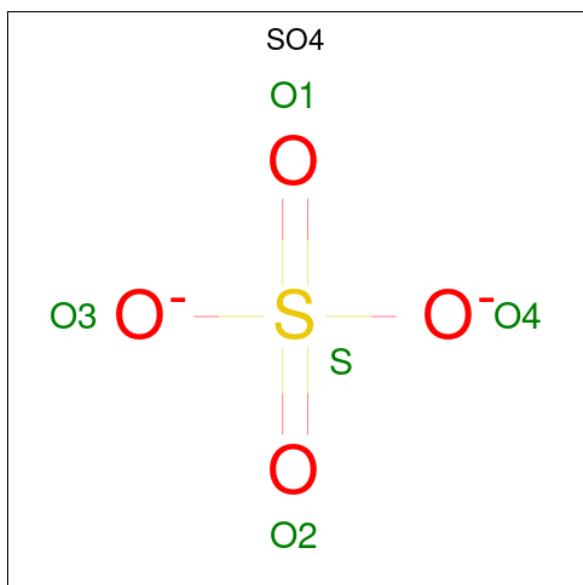
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	C	1	Total 6	C 3	O 3	0	0

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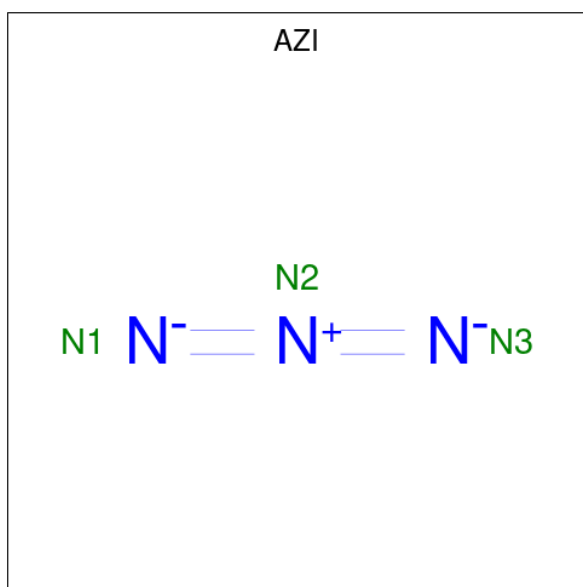
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N 3 3	0	0
4	B	1	Total N 3 3	0	0
4	C	1	Total N 3 3	0	0
4	C	1	Total N 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	80	Total O 80 80	0	0
5	B	87	Total O 87 87	0	0
5	C	98	Total O 98 98	0	0

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### 3 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.71Å 110.93Å 134.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.30 – 2.25 46.63 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (64.30-2.25) 100.0 (46.63-2.25)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.48 (at 2.24Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.191 , 0.226 0.188 , 0.191	Depositor DCC
$R_{free}$ test set	1394 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtrriage
Anisotropy	0.090	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4180	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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.

## 4 Model quality [i](#)

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

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### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	1172	-	4,4,4	0.36	0	6,6,6	0.23	0
2	GOL	B	1170	-	5,5,5	4.24	5 (100%)	5,5,5	0.50	0
4	AZI	C	1177	-	0,2,2	-	-	0,1,1	-	-
3	SO4	C	1175	-	4,4,4	0.34	0	6,6,6	0.23	0
4	AZI	A	1174	-	0,2,2	-	-	0,1,1	-	-
2	GOL	A	1171	-	5,5,5	4.44	5 (100%)	5,5,5	0.40	0
2	GOL	C	1172	-	5,5,5	4.23	5 (100%)	5,5,5	0.41	0
2	GOL	C	1171	-	5,5,5	4.19	5 (100%)	5,5,5	0.35	0
4	AZI	B	1173	-	0,2,2	-	-	0,1,1	-	-
4	AZI	C	1176	-	0,2,2	-	-	0,1,1	-	-
3	SO4	B	1171	-	4,4,4	0.30	0	6,6,6	0.20	0
3	SO4	A	1173	-	4,4,4	0.39	0	6,6,6	0.16	0
2	GOL	C	1173	-	5,5,5	4.15	5 (100%)	5,5,5	0.33	0
3	SO4	A	1172	-	4,4,4	0.26	0	6,6,6	0.28	0
3	SO4	C	1174	-	4,4,4	0.38	0	6,6,6	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	1170	-	-	2/4/4/4	-
2	GOL	A	1171	-	-	2/4/4/4	-
2	GOL	C	1172	-	-	4/4/4/4	-
2	GOL	C	1171	-	-	2/4/4/4	-
2	GOL	C	1173	-	-	1/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1172	GOL	C3-C2	-6.96	1.23	1.51
2	A	1171	GOL	C3-C2	-6.93	1.23	1.51
2	C	1171	GOL	C3-C2	-6.78	1.23	1.51
2	C	1173	GOL	C3-C2	-6.56	1.24	1.51
2	B	1170	GOL	C3-C2	-6.44	1.25	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1170	GOL	O1-C1	4.43	1.61	1.42
2	C	1173	GOL	O1-C1	4.25	1.60	1.42
2	A	1171	GOL	O1-C1	4.22	1.60	1.42
2	C	1172	GOL	O1-C1	4.14	1.59	1.42
2	C	1171	GOL	O1-C1	3.91	1.58	1.42
2	C	1173	GOL	O3-C3	3.57	1.57	1.42
2	A	1171	GOL	O2-C2	-3.56	1.32	1.43
2	C	1171	GOL	O3-C3	3.56	1.57	1.42
2	B	1170	GOL	O3-C3	3.51	1.57	1.42
2	A	1171	GOL	O3-C3	3.42	1.56	1.42
2	C	1172	GOL	O3-C3	3.28	1.56	1.42
2	B	1170	GOL	O2-C2	-2.94	1.34	1.43
2	A	1171	GOL	C1-C2	-2.86	1.40	1.51
2	C	1171	GOL	C1-C2	-2.83	1.40	1.51
2	B	1170	GOL	C1-C2	-2.80	1.40	1.51
2	C	1172	GOL	C1-C2	-2.71	1.40	1.51
2	C	1173	GOL	O2-C2	-2.58	1.35	1.43
2	C	1172	GOL	O2-C2	-2.41	1.36	1.43
2	C	1171	GOL	O2-C2	-2.39	1.36	1.43
2	C	1173	GOL	C1-C2	-2.39	1.41	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1170	GOL	C1-C2-C3-O3
2	C	1171	GOL	C1-C2-C3-O3
2	C	1171	GOL	O2-C2-C3-O3
2	C	1172	GOL	O1-C1-C2-C3
2	C	1172	GOL	C1-C2-C3-O3
2	A	1171	GOL	O1-C1-C2-C3
2	B	1170	GOL	O2-C2-C3-O3
2	C	1172	GOL	O1-C1-C2-O2
2	C	1172	GOL	O2-C2-C3-O3
2	A	1171	GOL	O1-C1-C2-O2
2	C	1173	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 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	163/177 (92%)	-0.05	4 (2%) 57 60	20, 31, 64, 73	0
1	B	163/177 (92%)	-0.11	9 (5%) 25 27	20, 31, 58, 69	0
1	C	165/177 (93%)	-0.21	2 (1%) 79 81	19, 31, 58, 67	0
All	All	491/531 (92%)	-0.13	15 (3%) 49 52	19, 31, 60, 73	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	HIS	3.8
1	B	50	HIS	3.8
1	C	97	TRP	3.7
1	C	50	HIS	3.5
1	A	97	TRP	3.5
1	A	42	VAL	2.8
1	B	7	THR	2.7
1	B	67	GLY	2.6
1	B	97	TRP	2.5
1	B	43	GLU	2.5
1	B	6	PRO	2.5
1	A	7	THR	2.4
1	B	15	GLU	2.2
1	B	42	VAL	2.0
1	B	66	GLN	2.0

### 5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.4 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
4	AZI	C	1177	3/3	0.83	0.15	53,53,54,54	0
2	GOL	C	1173	6/6	0.84	0.13	60,60,61,61	0
2	GOL	B	1170	6/6	0.84	0.15	65,66,67,67	0
2	GOL	C	1171	6/6	0.86	0.18	36,43,45,45	0
2	GOL	C	1172	6/6	0.88	0.20	46,47,47,48	0
4	AZI	B	1173	3/3	0.89	0.24	51,51,53,53	0
4	AZI	C	1176	3/3	0.92	0.09	49,49,50,50	0
2	GOL	A	1171	6/6	0.93	0.22	43,44,47,48	0
3	SO4	C	1174	5/5	0.97	0.09	53,53,54,55	0
3	SO4	A	1173	5/5	0.97	0.09	59,60,60,60	0
3	SO4	B	1171	5/5	0.97	0.14	44,45,47,48	0
3	SO4	B	1172	5/5	0.97	0.15	54,55,56,57	0
4	AZI	A	1174	3/3	0.98	0.17	44,44,44,45	0
3	SO4	C	1175	5/5	0.98	0.14	50,50,53,53	0
3	SO4	A	1172	5/5	0.99	0.10	31,32,33,34	0

### 5.5 Other polymers [i](#)

There are no such residues in this entry.